THE MECHANICS AND PHYSICS OF HIGH SPEED DISLOCATIONS: A CRITICAL REVIEW

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B. Gurrutxaga–Lerma[1,2], J. Verschueren[3], A. P. Sutton[4], and D. Dini[5]

[1]School of Metallurgy and Materials, University of Birmingham, B15 2TT Birmingham, UK
[2]Trinity College, University of Cambridge, CB2 1TQ Cambridge, UK
[3]Department of Materials, Imperial College London, SW7 2AZ London, UK
[4]Department of Physics, Imperial College London, SW7 2AZ London, UK
[5]Department of Mechanical Engineering, Imperial College London, SW7 2AZ London, UK

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Abstract

High speed dislocations have long been identified as the dominant feature governing the plastic response of crystalline materials subjected to high strain rates. They allegedly control deformation and failure response of industrial processes in a large range of applications, including machining, laser shock peening, punching, drilling, crashworthiness, foreign object damage,etc. Despite decades of study, achieving a consensus on the role and influence high speed dislocations have on the materials response observed at the macro-scale by the means of rigorous mechanistic grounding remains elusive. This article reviews both experimental and theoretical efforts made to address this issue in a systematic way. The lack of experimental evidence and direct observation of high speed dislocations means that most work on the matter is rooted on theory and simulations. This article offers a critical review of the competing theoretical accounts of high speed mechanisms, their underlying hypothesis, insights, and shortcomings. It explores the role that the speed of sound plays in the modelling of high speed dislocations, the way dislocations are modelled in the elastic continuum and how this approach can be used to study plasticity at high strain rates. The role atomistic models of dislocations have played in clarifying high speed motion mechanisms, and how they have led to the development of dislocation velocity-stress relations describing dislocation mobility is then also discussed. The article also reviews modelling efforts aimed at describing high speed dislocation mobility, and how different proposed physical mechanisms believed influence the motion. The article closes with an overview of the current state of the art and suggestions for key developments needed to improve our fundamental understanding in future research.

1 Introduction

What happens to a dislocation when it moves at velocities comparable to the speeds of sound of the material in which it propagates? Moving dislocations dominate the plastic deformation of crystalline materials[1]; thus, an adequate answer to this question would enable a better understanding and a more accurate physical modelling of many dislocation-mediated processes, where high speed dislocations are thought to be present. Such processes include moderate and high strain rate plasticity[2, 3], adiabatic shear banding[4], dynamic fracture[5], and many others. In turn, these mechanisms are known to dominate the mechanical response of industrially relevant processes, such as e.g. foreign object damage in the aerospace industry, machining[6], forging[7], laser shock peening[8] and wear[9]. Unfortunately, the field of high speed dislocation dynamics has been at the centre of debates and controversies since it was first posed in 1949[10, 11], and remains a research area with many mysteries and a salient absence of physical consensus. This is not due to a lack of effort: there have been attempts to tackle this from various viewpoints and employing many different methodologies, from continuum level elastodynamics to molecular dynamics. However, none of them have been able to provide a definitive, undisputed answer to the question posed above for two reasons.

First and foremost is the absence of experimental evidence caused by the technical challenges involved in generating and tracking dislocations at speeds of the order of kilometres per second. Admittedly, some related empirical results exist, such as the observation of supersonic cracks [12], twins [13] and dislocations in plasma crystals [14]. As will be discussed in section 2, these results notwithstanding, the direct experimental observations of fast moving dislocations in metals have been limited to velocities below about one third of the shear wave speed of the material [15, 16, 17, 18, 19, 20, 21], the lower boundary of the velocity regime of interest.

The second reason for the enduring uncertainty in this field stems from the multiplicity of theoretical and computational methods that have been employed to study fast moving dislocations. Without the guidance of unambiguous experimental evidence, advances in the field have been necessarily left to theoretical models and computer simulations. Generally speaking, the former take the form of linearly elastic continuum models at microsecond and micrometer time and length scales, in which the atomic nature of matter is neglected. These were some of the oldest and most successful models in micro- and defect mechanics [22, 1]. However, as will be shown in section 3, it quickly became apparent that the assumed description of the dislocation core, which needs to be added explicitly in these models, had significant impact on the derived results.

This motivated the atomistic[1] modelling of gliding dislocations, which will be discussed in section 4. These models captured the interaction between the dislocation and the lattice explicitly and, as such, complemented their continuum counterparts. The earliest atomistic models[23, 24, 25] were not given much consideration as they were limited to arguably oversimplified systems due to computational cost limitations. Furthermore, they contained instabilities at speeds below about half of the shear wave speed of the material which remained unexplained[24, 26, 25]. These instabilities were interpreted to mean that low velocity dislocation motion was impossible (cf. section 4.1). With the advent of the non-equilibrium molecular dynamics method, more realistic atomistic simulations were performed. Nowadays, computational resources are such that these simulations can be performed with plausible interaction potentials and adequate system sizes. However, they have so far not provided the field with the conclusive mechanistic understanding it yearns for because observations in these computer experiments showed little transferability to seemingly equivalent simulations, as will be discussed in section 4.

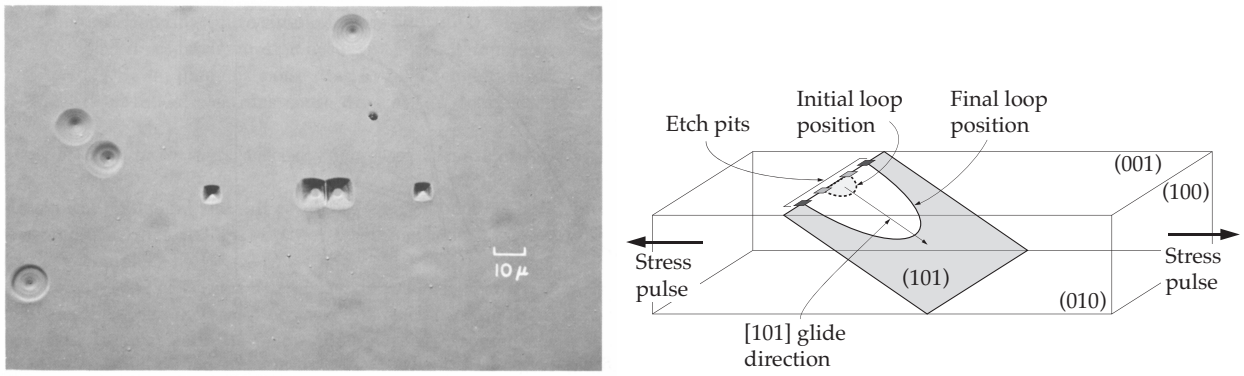
The study of high speed dislocations is motivated by the perceived need to explain physical phenomena where it has long been speculated that high speed, perhaps even supersonic, dislocations play a significant and necessary role. The paradigmatic example of this is shock loading: as stated for instance by Stroh[27] '*... it seems unlikely that dislocations move with so high a velocity, except possibly at the very highest strain rates, which may occur in explosive loading.*' Early attempts at explaining the plastic relaxation of a shock front, such as the Smith-Hornbogen model[28, 29], did indeed require dislocations to travel at supersonic speeds to trail the advancing shock front[2]. However, given that models such as the one proposed by Smith and Hornbogen failed to correctly predict the observed dislocation densities[2] and that by then supersonic dislocations were already seen as contentious[30], these attempts were quickly superseded by more sophisticated accounts[31, 32, 33, 34] that shifted the cause of plastic relaxation in shock loading from moving dislocations to dislocation generation behind the front[30]. These models were more consistent with the observed increase in dislocation density behind the shock front[31, 35, 36, 34, 30], whilst simultaneously requiring dislocations to move at subsonic speeds[34]. Thus, supersonic dislocations sparked remarkable research aimed at explaining physical phenomena by, paradoxically, explicitly seeking to avoid them. What also transpired is a lack of physical motivation for high speed dislocations: if they are not needed in shock loading, what are they for?

In fact, another important reason to study high speed dislocations is the description of dislocation *mobility*. Theoretical studies of high speed dislocations, which are experimentally unreachable, allow to define 'stress-velocity' *mobility laws*, which concern the theoretical relationship between the kinematic state of the dislocation (e.g., its glide speed v, or its acceleration) and the applied stimuli that drive the motion, usually captured via the Peach-Koehler force[37, 38] as a resolved shear stress τ acting on the dislocation. Mobility laws are particularly important because the macroscopic plastic flow is understood to be proportional to the average speed of dislocations[39]. As will be discussed in section 5, the emphasis the field places on whether the speeds of sound are a *limiting speed* to dislocation motion largely reflects the desire of reaching an adequate mobility law at high speeds, rather than explain specific macroscopic phenomena. Many of the theoretical discrepancies afflicting the field are also reflected in the search for a universally valid mobility law.

In this review, we will argue that the state of the field is such that we are still debating how fast moving dislocations should behave on a qualitative level. In section 2, the experimental evidence surrounding high speed dislocations is reviewed. Section 3 concerns continuum level models of high speed dislocation. Atomistic models are discussed in section 4. Section 5 discusses the many physical aspects affecting the description of high speed dislocation mobility.

[1] The term *atomistic* is used as a shorthand for "on the atomic scale" throughout.

[2] The Smith-Hornbogen dislocations are supersonic because they move obliquely at an angle θ behind the front, so they must reach speeds of $c_l/cos\theta$ to keep up with the front.



(a) Moving dislocation etch pits in LiF. Reproduced with permission from Gilman[47].

(b) Schematic of the motion of dislocations in an etch pit experiment. After [47].

Figure 1: Movement of dislocation etch pit in LiF under the application of an external stress pulse.

Section 6 closes the review with the conclusions and provides a critical outlook, particularly emphasising three areas in which progress is still needed to resolve long-standing issues in this fascinating research field.

2 Experimental evidence

The first experimental evidence of dislocations in motion was provided by Leibfried in 1950 [40]. In creep tests he showed that the experimental sample extended by about 0.1μm over timescales of about a second. Subsequently, he was able to ascribe this observation to moving dislocations [41], allowing him to estimate dislocation speeds of the order of 1m/s.[3] Subsequent studies also relied on indirect evidence, particularly from the growth of slip bands in aluminium [42, 43], reporting average dislocation speeds of no more than 200m/s [43]. Slip band growth has subsequently been used to estimate dislocation speeds, e.g., in bcc Fe [44], Fe-Si[45], or bcc Mo[46].

In the late '50s, direct evidence of dislocation mobility was provided by Gilman and Johnston [48, 15]. In their experiments of selective etching in LiF, Gilman and Johnston tracked the position of surface etch pits before and after a stress pulse had been applied on the sample (see fig.1). Whilst prior experiments could only infer dislocation speeds as averages over time and a large number of dislocations, selective etching enabled Gilman and Johnston to obtain the average speed of individual dislocations as the ratio between the distance moved by the pits and the duration of the stress pulse. By repeating the experiment at different applied stress levels, Gilman and Johnston constructed direct empirical evidence relating the applied stress to the average speed of individual dislocations[49], and of dislocation generation rates[49]. Their original results in LiF probed dislocation speeds spanning more than 10 orders of magnitude. They suggested the presence of a linear regime at low speeds and that velocity tended to saturate with increasing stress. Further selective etch experiments in the next decades replicated these results in a vast number of materials, under different temperature ranges and under irradiation conditions [50]. Materials tested in this way include the metals W [51], Fe [44, 52], Fe-C [53], Fe-Si [16, 54, 55], Al [56], Cu [57, 58, 59, 60], irradiated Cu[61], Al-Cu alloys [17, 21, 57, 62], Ni [63], Pb [64], Mg [65], Zn [66, 67, 68, 59, 69, 70, 71, 72], Nb [73, 74, 75], α-Ti [76], In [77], K [52], Mo [65, 78, 79], Ag [80], and a number of ceramics and semiconductors, including pure Ge [81] and Si [82, 83], LiF [48, 84, 85, 86], BeO [87], KCl [88], NaCl [89], KBr [90, 91], InSb [82, 92], GaAs [93], GaSb [82], InP [94], GeSi [95, 96]. In Si, particular focus was placed on studying the mobility of dislocations under various temperatures and doping conditions, often with seemingly contradictory results [82, 97, 98, 99, 100, 101, 102, 103, 104, 105]. By the 1960s most *in-situ* measurements of dislocation had progressed to using X-ray microscopy [103, 106, 107].

In parallel to the development of the selective etching technique, Granato and Stern [108] developed an alternative approach to estimating the *drag coefficient* of a moving dislocation based on the attenuation of sound waves in metals. This approach, commonly called the *stress relaxation technique*, built on theoretical work by Read [109] and Koehler [38]. The former associated the attenuation of stress waves to the presence of dislocations [109]. The latter then showed that this attenuation was inversely proportional to damping of the vibrations of pinned dislocation segments due to a drag-like force[38]. This 'drag-like' force f_{drag} is linearly proportional to the dislocation segment's own speed $f_{\text{drag}} = d \cdot v$, with d the drag coefficient[1]. Granato and Stern measured the attenuation rate and estimated values for

[3]This speed represents the collective average of the *drift speed* of the many dislocations involved in dislocation creep. Individual dislocations may move much faster than 1m/s, but be held at obstacles for significant periods of time.

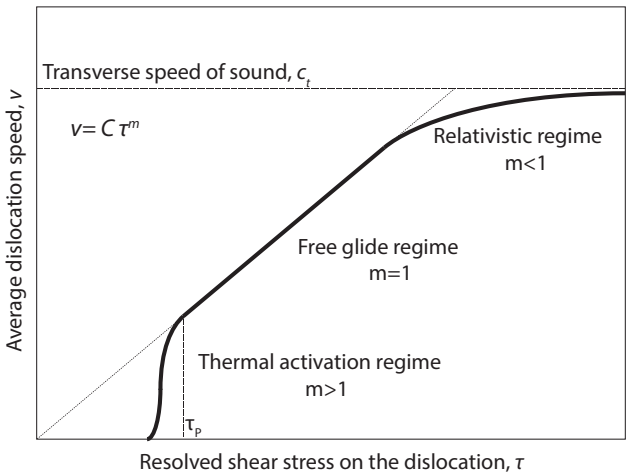


Figure 2: Classical representation of the three regimes of motion experienced by a glissile dislocation. For low speed and stress levels, dislocation motion is thermally activated (e.g., via the kink-pair mechanism[1]). Eventually the applied stress level overcomes the Peierls barrier τ_P, and the free glide regime is reached. As the dislocation's speed approaches the transverse speed of sound, dislocation speed is expected to saturate towards in the so-called 'relativistic' regime. Figure adapted from [138].

this drag-like force [108]. Using this technique, the 'canonical' values of the linear drag coefficients of a number of materials were obtained, including LiF [110], NaCl [111], KCl [110], Cu [112, 108, 110], Cu-Mn alloys [110], Al[19], Pb [113], Cd [114], Ta [115] and solid He [116, 117].

Dislocation velocity can also be measured using *in-situ* transmission electron microscopy (TEM), although this tends to limit the scope of the studies to extremely low average speeds (of the order of 10^{-6}m/s), often for groups of dislocations. Therefore, the approach is particularly suitable to study the kinetics of dislocation motion and the activation of different glide mechanisms under varied loading conditions. For instance, Shih et al. [118] measured speeds of 50nm/s for dislocations subjected to a constant strain rate in α-Ti, which increased to 70nm/s under the presence of hydrogen. Equally, Caillard [119, 120] reported average speeds of the order of 100nm/s for screw dislocations in pure Fe achieved by in-situ straining of the samples. A wide range of studies of this type exist, e.g. [121, 122, 123, 124, 125, 126], mostly focused on descriptions of glide in specific crystallographic orientations (see for instance [127, 128, 129, 130]) at very low, often unreported, speeds. Scanning electron microscopy (SEM) techniques have also been employed in a similar fashion, leading to equally low estimates of the average speeds [131].

Other experimental techniques have also been used to estimate dislocation velocities, usually relying on indirect evidence. For instance, Schaarwächter and Ebener [132] and Maass *et al.* [133] proposed using acoustic measurements to study the velocity of dislocation avalanches. Such indirect methods appear best suited to study effects related to work hardening and stage II-III plasticity [134], as they estimate velocities of the order of 1m/s in dense networks of dislocations. Taking advantage of the magnetoplastic effect, Kim et al. [135] were able to estimate dislocation speeds in Zn. Similar indirect measurements of dislocation mobility, based on correlating the macroscopic response with crystal plasticity laws reliant on dislocation drag expressions valid at very low speeds have been performed under restrictive loading conditions[136, 137]. These are discussed in greater detail in section 5.

2.1 The three regimes of dislocation motion

The aim of mobility experiments is to establish a relationship between the applied stress τ and the observed average dislocation velocity $\bar{v}$. This relationship or '*mobility law*' (see section 5 for more details) has commonly been represented with a power law of the form $\bar{v} = C\tau^m$ where C is a constant[2, 139]. This power law is entirely phenomenological, and has no physical basis; indeed, some authors have favoured other fittings laws(cf.[47, 140]). Although results display vast variability between different materials, temperatures, and alloying conditions, a general consensus arose demarcating three 'mobility' regimes characterised by the power law's fitting exponent m (cf. [2, 47]) and depicted in fig.2. For low applied stresses, the power law exponent would be very large, considerably above $m > 1$ [139, 2]. This regime was ascribed to the thermal activation of motion[47, 138, 141]. As is shown in fig.3 for dislocations in KCl crystals of different levels of purity [88], the exponent m would decrease with increasing stress, eventually reaching a quasi-linear regime where $m \approx 1$. This regime is the '*viscous drag regime*' we discuss in the sequel. At the upper

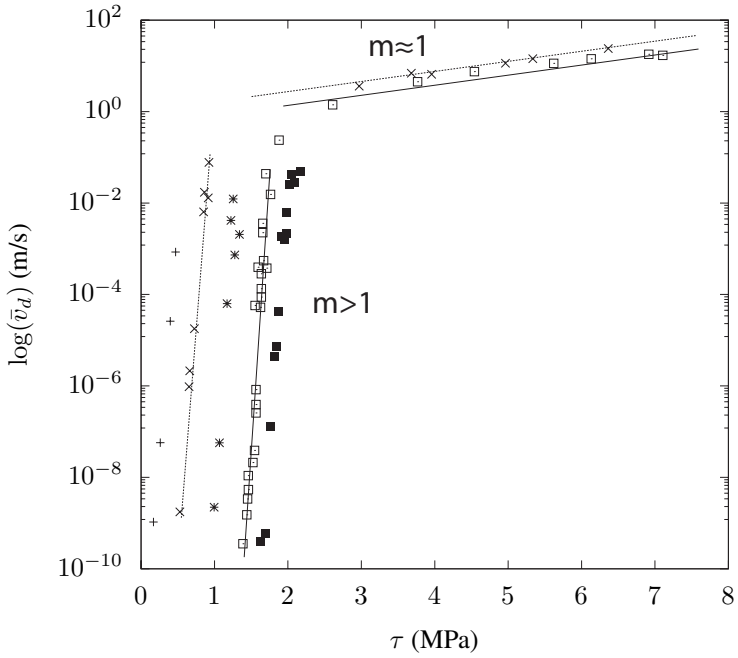


Figure 3: Mobility data for dislocations in KCl crystals of different purities, adapted from Lubenets and Startsev [88]. The data shows a clear change in the mobility as the free glide regime is reached.

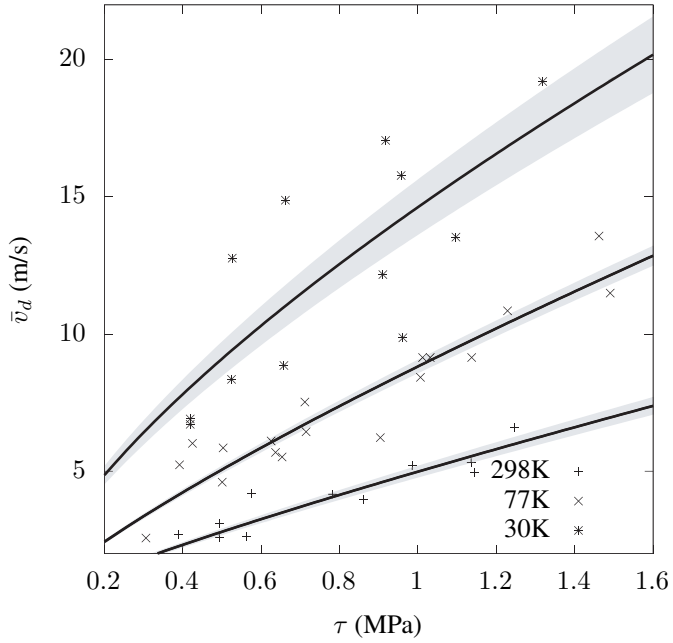


Figure 4: Selection of experimental data for the dislocation mobility in fcc Al at different temperatures, as reported by Parameswaran *et al.* [56]. The data has been fitted with a power law, that renders $\tau = 0.146\bar{v}^{1.197}$ for 298K, $\tau = 0.066\bar{v}^{1.247}$ for 77K, and $\tau = 0.02\bar{v}^{1.46}$ for 30K. An alternative data set may be found in Gorman *et al.* [19].

end, for high stresses and high speeds, the exponent was often reported to take values considerably below $m < 0.1$. For instance, Gilman reported values of $m = 0.05$[84] for LiF; Stein and Low gave values of $m = 0.022 - 0.028$ for Fe-Si[16]. At these high stresses, *relativistic effects* (see below) were said to dominate the motion[47, 140, 2].

The extraordinary non-linearities found for low and high speeds ($m \gg 1$ and $m \ll 1$, respectively) were often taken at face value [48, 16] and reported [139, 140, 2], despite the fact that non-linear scaling of that order is exceedingly rare [142]. This seems to suggest that this is the result of the inappropriate fitting via a power law of otherwise accountable physical behaviours. For instance, in studying the rate for kink-driven dislocation motion under applied stresses, Fitzgerald [143] has shown that the rationale for low speed non-linearities is to be found in the rate behaviour of the motion under small loads: exponential behaviours were being fitted with power laws. In the high speed regime, building on the approach introduced by Alshits and Indebon [50, 144], Blaschke [145, 146] has shown that the velocity of high speed dislocations saturates due to dislocation-phonon interactions, which result in an effective drag coefficient inversely proportional to powers of a rational function dependent on dislocation speed.

The $m \approx 1$ quasi-linear regime observed by Gilman and Johnston for LiF was corroborated by most subsequent experimental work. For instance, fig.4 shows etch-pit data obtained by Parameswaran *et al.* [56] for the mobility of dislocations in fcc Al at different temperatures. In this data set, the power law fit produces exponents m of order unity, consistent with the linear viscous regime measured in other materials. The existence of this regime agreed with theoretical work suggesting the existence of a 'drag' force proportional to the dislocation speed that dominated dislocation motion in the free glide regime [1] (see fig.2).

The presence of this drag force had been recognised early on by Leibfried [40], who was the first proponent of the *phonon scattering* effect that is thought to arise during the unobstructed glide of dislocations [138]. According to Leibfried [40], a phonon that would be transported unimpeded through a perfect lattice will be inelastically scattered by the dislocation's own elastic field, resulting in an energy loss that manifests as the dislocation glides in the form of a viscous drag acting on the dislocation. A considerable number of additional dispersion mechanisms have been proposed that may explain or contribute to explaining dislocation drag. These are discussed in greater detail in section 5.

The non-linear regime found at higher stresses in experiments was attributed to 'relativistic' effects [140, 47], because elastodynamics predicts that, in analogy to relativistic particles approaching the speed of light, the elastic energy of dislocations approaching at speeds close to the transverse speed of sound, c_t ought to diverge. This would entail a saturation in the $\tau \propto \bar{v}^m$ law as $\bar{b}$ approaches c_t (see section 3.3). In practice however, the speeds of dislocations in experiments where mobility laws have been determined are much less than those of the relativistic regime. In-situ experimental observations at speeds above $\approx 0.3c_t$ is, to the authors' knowledge, non-existent. The highest speeds reported come from Flinn and Tinder's work on etched LiF[147] and from Kumar and Clifton's[148] studies of slip band growth in LiF, where dislocations reaching $\approx$ 1100m/s are reported. Even at such speeds, the 'relativistic' Frank-Eshelby dislocation we discuss in detail in section 3.3 behaves almost like an elastostatic dislocation, as its elastic energy is only ≈ 1.05 times that at rest. The attribution of the observed non-linear regime to 'relativistic' effects appears spurious, and its explanation remains unclear.

Hitherto, *in-situ* studies of dislocation motion remain limited to low and moderate dislocation velocities. The number of crystalline systems that have been studied is limited, and many commonplace alloys of practical interest lack experimental studies of dislocation mobility, even at low speeds. The challenges for direct measurements of high speed dislocations are many: the loading rates at which they are expected to occur are accessible only through set-ups such as Hopkinson bar [149, 150], plate impact [151] or laser shock experiments [152] where *in-situ* microscopy is difficult. Equally, the required temporal and spatial resolution pushes current imaging capabilities to its limits, particularly for supersonic dislocations. Thus, most information about dislocation motion in the free glide and 'relativistic' regimes comes from theory and simulation.

3 Continuum models of gliding dislocations

The earliest models of high speed dislocations were founded on the continuum theory of linear elasticity. The speeds of sound play a central role in linear *elastodynamics*, where they represent the speeds at which information propagates in the form of (elastic) waves (cf.[153, 154]). The modelling of high speed dislocations in linear elasticity comes to depend critically on these speeds, because they entail that a dislocation travelling as fast as sound would require an infinite elastic energy. Thus, in elastodynamics the speeds of sound are commonly regarded as *limiting speeds* to dislocation motion – i.e., speeds that no dislocation may overcome. More sophisticated or physically insightful models produced subsequently tend not to regard the speeds of sound as limiting speeds (see section 4), even though for historical reasons the early insights offered by elastodynamics still dominate the way high speed dislocations are approached (e.g., 'high speed' dislocations are typically those moving at speeds approaching the transverse speed of sound, q.v.[155, 156, 157, 158, 159]).

This section aims to explain the whys and wherefores of these limiting speeds: why are the speeds of sound said to be limiting speeds to dislocation motion? What caveats are to be found in these models? What physical implications do they have? The crucial step to answer these questions is the derivation of the *elastodynamic* fields of moving dislocations.

3.1 General characteristics of the linear elastodynamic models of moving dislocations

All treatments of the elastodynamic fields of dislocations begin with their governing equation – the conservation of linear momentum – which, in terms of the displacement field in a linear elastic solid, are typically written as the Navier-Lamé equations[153],

$$\frac{1}{2}C_{ijkl}\left(u_{i,jj}(\mathbf{x},t)+u_{j,ij}(\mathbf{x},t)\right)=\rho\ddot{u}_i(\mathbf{x},t) \tag{1}$$

with repeated index denotes summation, u_i is the displacement vector, ρ the density, C_{ijkl} the elastic constant tensor, and $f_{,j}\equiv\partial_j f$.

For an isotropic solid it takes the form[154, 160]

$$(\lambda+\mu)u_{j,ji}(\mathbf{x},t)+\mu u_{i,jj}(\mathbf{x},t)=\rho\ddot{u}_i(\mathbf{x},t) \tag{2}$$

where λ and μ are Lamé's first parameter and the shear modulus, respectively, and ρ the density. Using the Kelvin potentials $\vec{\psi}\equiv\boldsymbol{\psi}$ and ϕ, the governing equations of linear elastodyamics can be uncoupled into two separate, monochromatic waves[161]:

$$\nabla^2\phi=\frac{1}{c_l^2}\frac{\partial^2\phi}{\partial t^2},\qquad \nabla^2\boldsymbol{\psi}=\frac{1}{c_t^2}\frac{\partial^2\boldsymbol{\psi}}{\partial t^2} \tag{3}$$

where

$$\mathbf{u}=\nabla\phi+\nabla\times\boldsymbol{\psi}\qquad u_i=\phi_{,j}+\epsilon_{ijk}\psi_{k,j} \tag{4}$$

and

$$c_t=\sqrt{\frac{\mu}{\rho}},\quad c_l=\sqrt{\frac{\lambda+2\mu}{\rho}} \tag{5}$$

are respectively the transverse and longitudinal speeds of sound, the speeds at which elastic fields propagate. This implies that in elastodynamics, information about a defect travels at well-defined, finite speeds.

3.2 The Frank-Eshelby dislocation: the uniformly moving Volterra dislocation in the steady state

The equation of motion for the displacement field of the uniformly moving Volterra screw dislocation in an isotropic continuum was first formulated in 1949 by Frank [10]. Frank started from eqn.2, which for the antiplane motions involved in the glide of screw dislocations, takes the form[154]:

$$\mu\nabla^2u_z(x,y,t)=\rho\frac{\partial^2u_z}{\partial t^2} \tag{6}$$

subjected to the boundary condition

$$u_z(x,0,t)=B\mathrm{H}(x-vt) \tag{7}$$

which models a Volterra screw dislocation with Burgers vector $(0,0,B)$ gliding along the x-axis at uniform speed v.

Frank's problem is a particularly simple case of the more general class of '*self-similar*' solutions known to exist in PDEs (cf.[162, 163, 164]). In this case, the spatial and temporal variables x and t appear in the boundary condition (eqn.7) in terms of $x-v\cdot t$, which leads to solutions of eqn.6 of the form

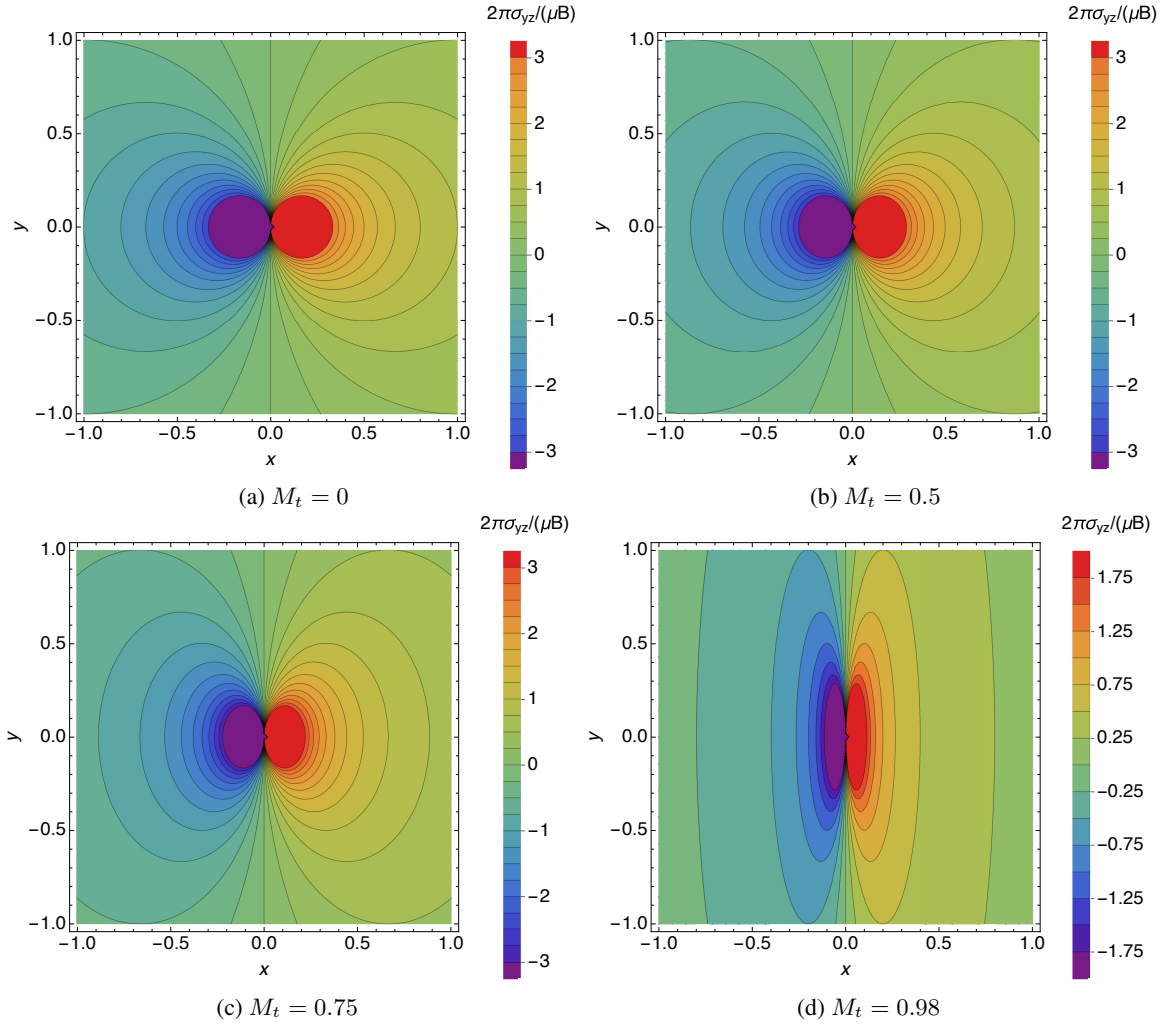
$$u_z(x,y,t)=u_z(x-vt,y) \tag{8}$$

This was explicitly achieved by Frank[10] by introducing a *Galilean transformation* to the independent variables

$$x\mapsto X\equiv x-vt,\qquad y\mapsto Y,\qquad t\mapsto T \tag{9}$$

In this particular case, this transformation group not only leads to a similarity solution, but reduces the number of independent variables from 3 to 2. Indeed, applying eqn.9 to eqn.6 reduces the problem to an analogue to the elastostatic problem:

$$\frac{1}{\gamma_t^2}\frac{\partial^2u_z}{\partial X^2}+\frac{\partial^2u_z}{\partial Y^2}=0,\qquad u_z(X)=B\mathrm{H}(X), \tag{10}$$



(a) $M_t = 0$ (b) $M_t = 0.5$

(c) $M_t = 0.75$ (d) $M_t = 0.98$

Figure 5: The σ_{yz} shear stress field of Frank's steady state screw dislocation[10], at different values of $M_t = v/c_t$. As may be seen, the solution tends to contract in the direction perpendicular to the motion as $M_t \to 1$.

the solution to which is the static field of a screw dislocation (q.v.[1]), which once the Galilean transformation is undone is of the form:

$$u_z(x, y, t) = \frac{B}{2\pi} \arctan\left[\frac{y}{\gamma_t(x - vt)}\right] \tag{11}$$

where $\gamma_t = (1 - v^2/c_t^2)^{-1/2}$ is a Lorentz factor with c_t the transverse speed of sound in the medium rather than the speed of light.

Eshelby also used a Galilean transformation to derive the equivalent solution for the uniformly moving Volterra edge dislocation[11]. Because the salient features of both solutions are analogous, we shall refer to this model as the '*Frank-Eshelby*' (FE) dislocation.

As is well-known[163, 165], solutions of the form eqn.11 (i.e., of the form of $u_z(x, y, t) = u_z(x - vt, y)$), describe a *plane wave* or *traveling wave* of velocity v and profile u_z in the x direction. This travelling wave only serves to model a uniformly moving dislocation that has moved in this manner ever since $t \to -\infty$. This arguably does not happen in reality, where at the very least a dislocation will accelerate from rest. The interest of the FE solution lies in that, as other self-similar solutions, it is an 'attractor'(cf.[166],p.51) for the *transient* motions of the dislocation, which would be modelled with a different set of boundary conditions (see section 3.3) and have far more contrived analytical solutions. Thus, it may be regarded as the *steady state* solution that a transient motion would tend to. As a result, the main purpose of the FE dislocation is not in accurately modelling dislocation motion, but in identifying the formation of singularities after the effects of the transient motions have faded.

One of the main properties of self-similar solutions is that the energy is a constant of the motion[163] – to put it otherwise, the traveling wave does not radiate energy. Frank for instance showed that the elastic energy E associated with the uniformly moving screw dislocation is[10]

$$E = \gamma_t E_0 \tag{12}$$

As may be seen in eqn.12, as $v \to c_t$, then $\gamma_t \to \infty$, whereupon a strong singularity appears to arise when the screw dislocation moves at the transverse speed of sound. Eshelby's[11] analysis for edge dislocations shows that their elastic energy is equally invariant, and that it diverges both at c_t and c_l.

This singularity was evocative of relativistic particles approaching the speed of light, a connection not missed by Frank and Eshelby[10, 11]. It naturally lead to the conclusion that the speed of sound is a *limiting speed* for moving dislocations, as it would require an infinitely large energy to accelerate dislocations beyond these velocities of infinite elastic self-energy [11]. In addition, Eshelby also discovered a "radiation free state" affecting edge dislocations gliding with velocity $\sqrt{2}c_t$, for which the required driving force to maintain uniform motion of the dislocation was zero [11]. Eshelby was quick to draw attention to the fact that the route to this state seemed to be obstructed by the hard barrier for gliding edges at c_t.

The divergence as $v \to c_t$ also manifests itself in the stress fields of the dislocation, which for the screw dislocation are given by[10]

$$\begin{aligned} \sigma_{xz} &= -\frac{\mu B}{2\pi}\frac{y}{y^2+\gamma_t^2(x-vt)^2} \\ \sigma_{yz} &= \frac{\mu B}{2\pi}\frac{\gamma_t(x-vt)}{y^2+\gamma_t^2(x-vt)^2} \end{aligned} \tag{13}$$

Clearly, as $v \to c_t$ both stress fields tend to vanish. Interestingly however, as $v \to c_t$, they both *contract* along the x direction. This is shown in fig.5, where it may be seen that this contraction is barely noticeable until around $v \approx 0.75c_t$, but very marked for dislocations gliding with speeds very close to c_t. To Frank and Eshelby[10, 11], this was evocative of the *Fitzgerald contraction* that relativistic electric charges are known to display[165].

Thus, the singularities observed at the speed of sound appeared to be in complete analogy to the divergences that arise in the fundamental equations of special relativity as a particle's velocity approaches the speed of light. They were quickly ascribed to a '*relativistic*' effect[167, 168], a loose terminology that has become pervasive in the literature.[4]. In fact, the relativistic picture of dislocation dynamics was formally laid out by Eshelby in 1953 using an "electromagnetic analogy" which attempted to describe the dynamics of dislocations in the language of electrodynamics[169]. However, it was shown later that the equivalent Lorentz force was irrelevant for moving dislocations [170, 22] (see also section 5). Only then was it accepted that the analogy between electromagnetism and dislocation theory was inappropriate.

Nevertheless, the notion that relativistic effects somehow govern dislocation motion was reinforced by Cottrell[167], Weertman[171], Hirth and Lothe[1], Teodosiu[172] and Gilman[47], amongst others, who reworked Frank and Eshelby's original derivations, preferring to explicitly invoke a Lorentz transformation instead:

$$x \mapsto X' \equiv \frac{x-vt}{\sqrt{1-\frac{v^2}{c_t^2}}}, \qquad y \mapsto Y', \qquad t \mapsto T' \equiv \frac{t-x\frac{v}{c_t^2}}{\sqrt{1-\frac{v^2}{c_t^2}}} \tag{14}$$

For $v =$ constant, the Lorentz transformation reduces eqn.6 to

$$\frac{\partial^2 u_z}{\partial X'^2} + \frac{\partial^2 u_z}{\partial Y'^2} = 0, \qquad u_z(X') = B\mathrm{H}(X'/\gamma_t), \tag{15}$$

The solution is again eqn.11.

Despite its initial popularity, there are good reasons to have reservations about the seemingly close connection between special relativity and dislocation dynamics as there seems to be little physical motivation behind it. Elastodynamic solutions are, after all, solutions to Newton's equations of motion, and cannot be expected to obey the limiting premises of special relativity. As we have discussed, the FE solution is just a traveling wave solution, which could be regarded as the *steady state* solution to more general motions. Its main purpose is in successfully identifying singular behaviours. The fact that the steady state field of a uniformly moving straight dislocation could be solved by applying a Lorentz transform to the static equation is not in itself surprising because the governing equation takes the form of a wave equation [10], which are Lorentz invariant [165, 163]. However, the introduction of the Lorentz transformation has

[4] See for instance Nabarro[140],p.491; or Hirth and Lothe [1], Ch.7; Meyers[2], Ch.13.

a number of disconcerting implications. First, it appears to be unnecessary: a Galilean transformation achieves the same solution. Second, the time dilation property attached to the Lorentz transformation seems extraneous in a classical context, so much so that Hirth and Lothe [1] perfunctorily dismissed it as having '*no deep significance*'. After all, what can a time contraction associated with the moving dislocation possibly mean? Third, this methodology ascribes the same physical importance to the speed of sound in a medium as to the speed of light has in vacuum. This would lead one to conclude that the speed of sound in any medium would be an insurmountable barrier, a conclusion which is known to false: supersonic cracks, for instance, are empirically attested[12]. Finally, the application of methods borne out of special relativity to dislocation dynamics tacitly assumes that the speed of sound is constant across all moving reference frames; this cannot be true as sound necessarily propagates in a medium.[161]

3.2.1 Frenkel-Kontorova models

The FE relativistic dislocation finds an analogue in the Frenkel-Kontorova (FK) model of dislocation motion[173, 174]. In the FK model, the dislocation line or, more properly, the dislocation core, forms part of a one-dimensional chain of atoms. Each atom has mass m, interacts with its two nearest neighbours via an elastic force of spring constant k, and is subjected to a one-dimensional background sinusoidal potential energy of period λ and amplitude Λ. The moving dislocation is represented by a soliton that propagates across the chain of atoms. If u_n denotes the displacement away from the equilibrium position of the n^{th} atom in the chain, then linear momentum conservation requires that[140]

$$k\frac{\partial^2 u_n^2}{\partial x_n^2} - m\frac{\partial^2 u_n}{\partial t^2} = 2\pi\frac{\Lambda}{\lambda^2}\sin(2\pi u_n) \tag{16}$$

This non-linear hyperbolic PDE is well-known to have steady state and self-similar particular solutions[163]. In particular, if each soliton/dislocation moves with uniform speed v, then it becomes a plane wave $u_n = u_n(x_n - vt)$ (see [163], p.176), and the equation can be reduced to steady-state (stationary) form[140]:

$$k\left(1 - \frac{mv^2}{k\lambda^2}\right)\frac{\partial^2 u_n}{\partial x^2} = 2\pi\frac{\Lambda}{\lambda^2}\sin(2\pi u_n) \tag{17}$$

which is the same equation as that in the stationary case. The solution to this equation is well-known[175]. Crucially, in the steady state it entails a limiting speed

$$c_{FK} = \sqrt{\frac{k\lambda^2}{m}} \tag{18}$$

which happens to be the speed of small perturbations in the chain of atoms. Furthermore, the energy associated with an individual soliton-dislocation in the chain is a constant of the motion, $E = E_0/\sqrt{1 - v^2/c_{FK}^2}$ with E_0 the energy of the dislocation at rest, so it diverges at $v = c_{FK}$.

3.2.2 Shortcomings of self-similar models

That a traveling wave solution to a hyperbolic PDE displays singularities at the characteristic speeds of the medium is unsurprising: these are embedded into the mathematical structure of the problem[5]. The speed of sound therefore arises as an *ad hoc* limiting speed for linear elasticity. Indeed, the limiting speed of the FK model, c_{FK}, is different to the speeds of sound, but formally analogous.

In both the self-similar FE and FK solutions, the *hard barriers* to dislocation motion arise because the governing PDE problem happens to be symmetric under a specific set of transformations. Crucially, the hyperbolic PDE that governs both problems lacks dissipative terms[176], so they can develop shocks for perturbations travelling at the PDE's characteristic speeds[163]. Although shock waves are observed in solids as a matter of course (cf.[2, 177]), which would suggest that the description provided by linear elasticity ought to be acceptable, an open question remains as to whether additional dissipative mechanisms, or indeed the geometrical modelling of the dislocation core, play a role that may facilitate the motion of high speed dislocation. The question therefore becomes whether or not the underlying physics are correctly captured by either of these models, and whether the consequences of the symmetries in the governing PDE would remain largely unchanged if the latter were broken.

For the FK model, it seems clear that the answer is no. The FK model is a highly idealised abstraction: it does not include the elastic energy of the elastic continua on either side of the slip plane, and concentrates the misfit energy of the dislocation's core in the dislocation line itself, which is represented by a planar wave in the form of a compressive soliton travelling through a 1D chain of atoms. Although the FK model has many uses in studying kink-driven drift [178, 179], it can hardly represent adequately a dislocation in free glide.

[5]The energy of a travelling wave source moving at the characteristic speed cannot escape its source.

For the FE model of a moving dislocation, the answer is also no, but in a more nuanced way. Some of the physical approximations it entails are easy to identify: it relies on linear isotropic elasticity, so it will miss the non-linearities that may be relevant at the core or under the predicted divergences at the speeds of sound[11]; the Volterra dislocation it models has an infinitely thin core; it does not allow for dissipation or attenuation mechanisms in the dislocation motion; it models a travelling wave, so the dislocation operates in a steady state it cannot escape – there is neither acceleration nor deceleration.

Furthermore, both models fail to provide a feasible and universal model of dislocation mobility[169]: The relation between the geometrical description of the elastic field of a dislocation and the mobility of a dislocation at large remains far from clear, unless additional dissipative effects are accounted for. Indeed, under the application of a remote shear stress, and in the absence of any other physical mechanisms at play, a dislocation converting all the work of an applied stress into its elastic self-energy would reach the terminal speed of sound at applied stresses of less than 10 MPa, which does not agree with experimental reality.[167]

3.3 Elastodynamic models of transient motion

The study of *transient* elastodynamic effects affecting moving dislocations arises as a way of providing a more complete description of its elastodynamic fields, as well as a means of evaluating part of the energy radiated by the moving dislocation, in the form of acoustic waves[180]. Initially, this seemed to be targeted at the drag force on dislocations, which Leibfried[40] attributed to the '*sound waves* [that] *are scattered by the dislocation structure*'[6].

As with the Frank-Eshelby problem, the transient problem of elastodynamic dislocation motion is governed by the conservation of linear momentum (eqn.2), subjected to appropriate boundary conditions able to generate a transient motion. The solution procedure of transient elastodynamic problems, which are inherently hyperbolic, can differ greatly from their static, parabolic counterparts[163], and be of considerable sophistication[154, 153]. Building on the Green's function approach[181], Nabarro[182] paved the way for further developments in the field when he studied the injection ('*synthesis*') of an infinitesimal dislocation loop in an elastodynamic continuum, an early application of Leibfried's[183] distributed dislocation technique[22, 184]. Nabarro's solution is the fundamental solution (i.e., the Green's function) that would have to be convolved with the generally time-dependent shape function of the slip surface of a dislocation loop to attain the actual elastic fields of a moving dislocation. Nabarro[182] used this fundamental solution to recover the field of Frank's uniformly moving screw dislocation.

The potential of the Green's function approach was recognised by Mura[185], who derived to the authors' knowledge the first complete formulation of the displacement and velocity fields of an expanding dislocation loop. This solution enables a general description of the elastodynamic fields of a dislocation loop, whether *transient* or in the steady state. Mura's solution is in effect the elastodynamic extension to Volterra's formula for the field of a dislocation loop[1, 22], and it serves to describe the transient elastic field of a generally non-uniformly moving dislocation loop. In its general form, if $S(t)$ denotes the time-dependent slip surface enclosed by the loop, it is[185, 186]

$$u_p(\mathbf{x},t) = \int_{-\infty}^{t}\int_{S(t')} B_i \nu_j C_{ijkl} G_{kp,q}(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}S'\mathrm{d}t' \tag{19}$$

where $\mathbf{x} \in \mathbb{R}^3$, $G_{ij}(\mathbf{x},t)$ is the dynamic Green's function[181, 153, 22], B_i the loop's Burgers vector, and ν_j the slip surface normal.

Although it provides a complete representation of the fields of an arbitrarily expanding or contracting dislocation loop, Mura's dynamic formula (eqn.19) did not differ fundamentally from the basic insights of the Frank-Eshelby solution: it too displays singularities at the speed of sound, suggestive that a transient treatment of motion also forbids supersonic dislocations. It is also inherently difficult to handle. The convolution integral in eqn.19 depends on the arbitrary form for $S(t)$ [185] over each past time from $t' \to -\infty$ to $t' = t$. This indicates that the displacement field of a dislocation loop at any particular time is determined by where it was at all previous times. This links to Eshelby's famous dictum that '*the dislocation is haunted by its past*'[187]. Mura used eqn.19 to recover Frank's solution for the uniformly moving screw dislocation[188], and to investigate the fields of a vibrating screw dislocation[188, 189], a problem that had been studied by Eshelby[190] in connection to internal friction in metals. Thus, it seemed that a full elastodynamic treatment offered few new insights.

3.3.1 Geophysical models of moving dislocations

The introduction of aspects of the modern theory of dislocations to the study of seismological events in the late 1950s in seminal works by, amongst others, Steketee[191, 192] and Chinnery[193] stirred a great deal of interest in

[6] Our translation, [40].

dislocations as dynamic, expanding objects. Seismological dislocations need not represent Volterra disregistries in a classical crystallographic sense(cf.[194])[7]. Whereas the dynamic dislocation remained a largely specialist application in dislocation theory, in seismology it quickly became an object of utmost importance to be able to understand faulting[195, 196]. The aim was often to provide theoretical models for the 'primary' or 'pressure' P waves and 'secondary' or 'shear' S waves radiated by a seismological fault to infer the sources of seismological events[197, 196, 195]. These source are modelled at different levels of refinement as distributions of force or moment couples[198, 194, 199, 195, 197], dislocations[200, 201, 200], or more general extended defects[195]. In 1959 for instance, Knopoff and Gilbert[202] achieved closed-form solutions to the elastic field of a finite straight edge dislocation, and provided an analysis of their elastic fields similar to that derived later on by Markenscoff and Clifton[35]. That same year, Ang and Williams[203] used the Cagniard-de Hoop technique[204, 205] to solve the field of a uniformly moving general fault. Furthermore, independently from Mura[185], Dahlen[201] rigorously derived eqn.19 for the field of an arbitrarily expanding Volterra dislocation loop, and provided a thorough study of the energetics involved in their expansion[206], which was missing in Mura's[185, 188] treatment.

Many of the developments in seismology in the 1960s and 1970s provided an almost complete treatment of the planar elastodynamic dislocation. Building on Ang and Williams[203], Mitra[207] used the Cagniard-de Hoop technique to obtain the closed-form solution to the fields of a uniformly moving screw dislocation that begins its motion from rest. Based on previous work by Niazy[208] and by Boore[209], Boore and coworkers[210] derived the closed-form solutions to the elastic fields of a uniformly moving edge dislocation that begins its motion from rest. Remarkably, they already considered various generalisations to the problem, including the presence of free surfaces[210], and suggested refined models of the dislocation 'core' via a Peierls-Nabarro regularisation[209] and ramp cores of different kinds[210], showing that dislocations with finite-width cores avoided the singularities when the speed of sound was reached. Mitra's and Boore's solutions were further generalised by Geller[211] to allow for non-Volterra slip functions (see also [200]), thereby regularising the dislocation 'core'. Three dimensional studies of what is sometimes called '*Haskell's rectangular fault model*'[197], entailing the fundamental solution to an uniformly expanding rectangular dislocation loop, were also studied to model earthquake sources[212, 200, 213, 214, 215].

Studies of this sort largely remained unknown in the micromechanics community, and the solutions reported here would not be found in the micromechanics literature until the work of Markenscoff[216, 217]. The elastodynamic treatment of dislocations offered in seismology explored a number of features relevant to high speed dislocations. For one thing, the elastic fields of dislocations are being described as wave-like, propagating fields in finite times and displaying a host of features typical of acoustic sources, including Doppler ('Lorentz') contractions[210, 218], Mach cones[218], with strong asymmetries in the fields depending on the direction of motion, which were not present in the Frank-Eshelby steady state dislocations. Finally, they showed that the singularities found at the speeds of sound were related to the infinitely thin core of the Volterra dislocation, and could be avoided if the core had a finite width[209, 210].

3.3.2 Fully transient solutions to dislocation motion

Most of these features would finally be would finally be introduced into the micromechanics community in the early 1980s with the work of Markenscoff and coworkers[216, 217, 219]. In a series of articles, Markenscoff provided the complete closed-form solutions to the elastodynamic fields of straight screw [216] and edge[217] dislocations, and of loops[220]. These solutions, of considerable complexity compared to their elastostatic counterparts, describe the non-uniform motion of dislocations, and when particularised to uniform motions, reduce to the solutions achieved by Mitra[207] and Boore et al.[210]. The injection (creation) and non-uniform motion of dislocations requires an additional set of elastodynamic solutions derived by Jokl et al.[221] for screw dislocations, and by Gurrutxaga-Lerma et al.[222] for edge dislocations.

Similar to the seismological literature, the elastodynamic fields attained by Markenscoff and colleagues describe dislocations as wave sources in a linear elastic medium. Figure 6 reproduces the stress field of an injected, uniformly (a) and non-uniformly (b) moving edge dislocation. In both cases, the dislocation was injected at the origin at time $t = 0$, and proceeded to move with (a) uniform speed and (b) a random speed between zero and the transverse speed of sound over short time steps. In both cases, the elastic field consists of two wavefronts (propagating at the transverse and longitudinal speeds of sound). However, even if the two dislocation are at the same final position in (a) and (b), their fields differ from each very significantly. This is because of how they reached their final position differs. As a result, the interaction of the elastodynamic dislocation with its surrounding are markedly different from that of the elastostatic dislocation. If the edge dislocation is made to move at speeds approaching the transverse speed of sound, a marked contraction of the fields is observed which indicates that, as with the Frank-Eshelby travelling wave solutions, the elastic self-energy of the dislocation is expected to diverge at the sound barrier[35].

[7] Seismological dislocations need not have a quantised Burgers vector, may represent Somigliana dislocations, or even more general shear and compressive faults.

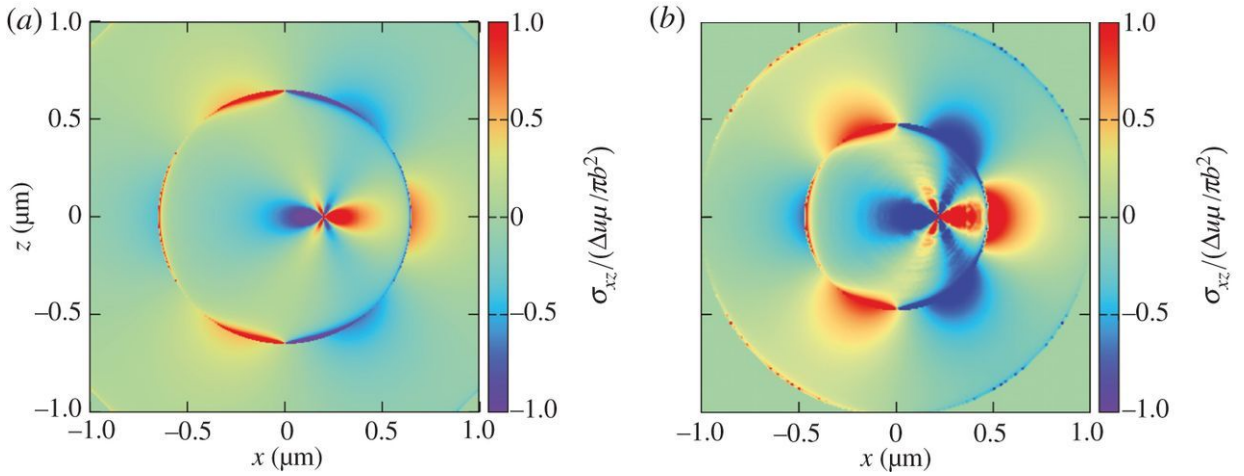


Figure 6: Elastodynamic σ_{xy} stress field component of an injected edge dislocation, from Gurrutxaga-Lerma et al.[222]. The dislocation was injected at $t = 0$ at the origin, and thereafter moved (a) with uniform speed; (b)with a random speed between $v \in (0, c_t)$ each time step. The stress field is made up of two separate monochromatic waves: one due to the longitudinal ('P') waves, which expands at c_l and is demarcated by the outer wave front in (b); and one due to the transverse ('S') waves, which expands at c_t and is demarcated by the inner wave front. Figure reproduced from Gurrutxaga-Lerma et al.[222] under CC BY 4.0.

3.3.3 Instabilities at the Rayleigh wave speed

Further theoretical aspects of high speed dislocations may be noted. In parallel to Markenscoff, Brock[223] derived a closed-form solution to the elastodynamic fields of a non-uniformly moving edge dislocation, which he expressed in terms of spatial derivatives rather than, as Markenscoff did, of time derivatives. In subsequent work, Brock[224] generalised the problem of a moving dislocation to arbitrary (i.e., not necessarily rectilinear) trajectories, which amongst other things enables the modelling of high speed climb, a solution that had previously been partially achieved by Burgers and Freund [225] as the fundamental solution to the propagation of a mode I crack. Brock also derived elastodynamic solutions for dislocation loops undergoing arbitrary motion [226].

In his analysis of the non-uniformly moving edge dislocation, Brock[223] noted that for dislocations gliding above the Rayleigh wave speed, c_R, there exists a reversal in the sign of the shear stress field that he linked to the presence of a potential limiting speed at c_R, below the transverse speed of sound.

The potential role of the Rayleigh wave speed as a limiting speed had already been noted by Weertman[227] in relation to Eshelby's solution to the uniformly moving edge dislocation. As with the elastodynamic case discussed by Brock[223], the shear stress component of Eshelby's solution also reverses signs for $v_d > c_R$. Weertman argued[227] that in that case, like-signed dislocations would attract one another, and it would become energetically favourable for them to cluster into groups of superdislocations. Weertman also showed[171] that a *kinematic generation* mechanism became possible, whereby a single edge dislocation gliding above the Rayleigh wave speed would dissociate into two like-signed dislocations and one unlike signed dislocation, conserving the total Burgers vector. Hirth and Lothe[1] linked this kinematic generation mechanism with Frank's[228] original ideas about the *kinematic* dislocation source, in which a dislocation would be able to generate new pairs by resonating with a free surface.

According to Weertman, if the kinetic energy of a moving dislocation is large enough, it may nucleate 2 dislocations of opposite sign [170] as sketched in fig.7, see e.g.[229, 171, 230, 231, 170, 1]. This may therefore be an important source of dislocations in high strain rate (upwards of $\sim 10^6 s^{-1}$) experiments and simulations [232]. At these strain rates, *homogeneous nucleation* - the generation of dislocations in complete absence of other defects or sources - was demonstrated to play an important role in both real [233, 234] and simulated shock experiments [235, 236, 237, 238, 234].

Although there are reasons to believe that this Rayleigh wave instability is a mathematical feature grounded in linear elasticity, its significance remains an open matter of research, and it might affect the interactions of high speed dislocations with free surfaces. In deriving the image forces for arbitrarily moving edge and screw dislocations in the presence of a planar free surface, Gurrutxaga-Lerma et al.[232] showed that an edge dislocation being drawn towards the free surface with speed greater than c_R would experience a repulsive image force. Under these conditions, if a dislocation were to be freely accelerated from rest under the sole action of the elastodynamic image force, it would never

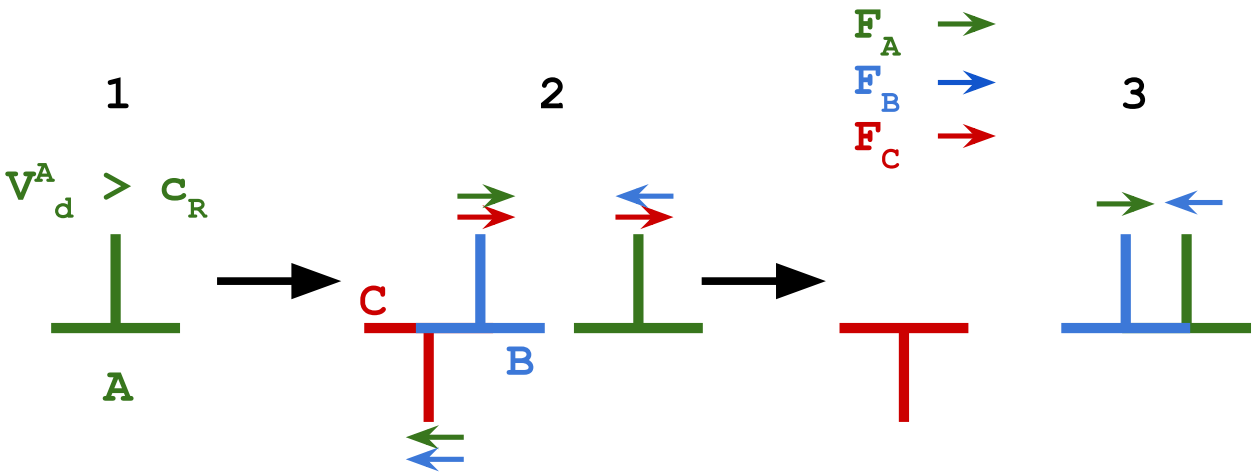


Figure 7: Schematic representation in three steps of the kinematic generation of edge dislocations according to continuum theory [1]. The colour of the arrow indicates the force created by the dislocation with the same colour. The vectors labelled F_A represent the forces on B and C due to A, and similarly for F_B and F_C. Step 1 shows an edge dislocation A travelling with a speed above the Rayleigh wave speed, which generates two nascent edge dislocations of opposite sign (B and C), shown in step 2. From the interactions between the dislocations represented in stage 2, it can be seen that this results in the final configuration consisting of a single dislocation C moving to the left, and a bound dislocation pair A and B moving to the right.

reach the free surface, or would be reflected by it. Although the significance of this effect remains largely unexplored, atomistic simulations by Li et al.[239] observed that high speed dislocations reaching a free surface were able to bounce back into the bulk, which they associated with strain bursts observed in nanopillars compressed with very high stresses.

The elastodynamic treatment of the image forces by Gurrutxaga-Lerma and coworkers[232, 240] showed a number of additional unexpected effects. The image force of a dislocation moving towards the free surface is dynamically magnified relative to the elastostatic solution. As reported by Gurrutxaga-Lerma et al.[232], the magnification appears to be very strong: a dislocation travelling at $\approx$ 100m/s sees its image force magnitude doubled within $1 - 5$ns. These speeds and timescales are easily achievable in low strain rate applications. The significance of this effect remains unexplored.

3.3.4 Regularising the dislocation core

After supersonic dislocations were first reported in molecular dynamics simulations[157], the apparent challenge to the existing consensus (we call it apparent because both Eshelby[169] and various lattice dynamics models had already discussed mechanisms whereby the transverse speed of sound would not constitute an upper limit on the speed of a dislocation[241, 242]) stimulated a number of elastodynamic studies to explain the discrepancy.

The main concern centred on the dislocation core. In studying the Peierls-Nabarro model of a moving dislocation Eshelby[169] noted that were the core to have a finite width, then '*a supersonic dislocation is a formal possibility.*' Boore and coworkers [209, 210] had reached similar conclusions when regularising the core of a uniformly moving seismological dislocation.

A first attempt at regularising the core via the Peirls-Nabarro (PN) model[243, 244] applied to high speed dislocations was put forward by Weertman [245]. He investigated the role of the assumed force law across the cut plane in the PN model for uniformly gliding screw and edge dislocations [245, 168, 170]. For screw dislocations he concluded that they are limited by the shear wave speed of the material, in agreement with Eshelby before him [180]. For the edge case however, Weertman argued that the traditional PN sinusoidal force law used by Eshelby was physically unsuitable [245], and examined alternatives. In so doing, Weertman concluded that edge dislocations could overcome c_t and that the limiting velocity was to be found somewhere in the transonic regime [245] (i.e., for dislocaito speeds above c_t but below c_l). However, like Eshelby before him, he too had to forgo definitive quantitative results admitting that these would be sensitive to the exact detail of the assumed force law in the PN core model [245].

Markenscoff and coworkers[246, 247, 248] recognised that as in the elastostatic case, the elastodynamic solutions contained a number of singularities directly related to the inadequate treatment of the core. They showed that if the core were to be spread out over a finite width in a ramp-like manner, the sound barrier due to the Mach wavefront may be

overcome[246, 247, 248]. Lazar treated the uniformly moving screw dislocation within an elastodynamic gauge theory for dislocations which removed the usual divergences near the Volterra dislocation core [249]. He found no objections to supersonic screw dislocations [249]. Equally so, Acharya and collaborators [250, 251], using a sophisticated large strain formulation [252, 253], upheld the possibility of supersonic dislocations.

Finally, Pellegrini provided the most complete continuum treatment of high speed dislocation to date with a fully elastodynamic treatment of the moving PN dislocation [254, 255, 256, 257]. Building on previous work by Pillon *et al.* [258], he proposed a method to solve the dynamic Peierls-Nabarro equations which had been derived previously but never solved due to their inherent mathematical complexity [169]. This so-called collective variable approach did not constrain the core's dynamics a priori, as was the case for most dynamic PN models before him. In contrast, the dynamics of the core was solved for explicitly as part of the solution scheme [256, 257]. He ultimately concluded that transient transonic motion for edge dislocations may be possible [257]. However, the model remained inconclusive with regards to the possibility of uniform motion in the transonic (above c_t but below c_l) and supersonic (above c_l) regimes [257].

Further models aimed at regularising the dislocation's core have been proposed [259, 260, 261, 262], favouring the possibility of transonic motions. The theoretical impossibility of supersonic dislocations is, broadly speaking, attributed to the use of linear elasticity[263, 253, 261] and the infinitely thin core of Volterra dislocations[264, 257, 249, 253].

3.4 Retardation effects and shock loading

When studying the influence of high speed dislocations, focus is usually placed on the way dislocation mobility itself is affected at high speeds (e.g., [1, 265, 266, 267]). What the actual effect high speed dislocations have in the mechanical response of materials has not received anywhere near the same level of attention. It is in fact common to treat the fields of the moving dislocations elastostatically, even though the finite time taken for their elastic fields to propagate may have significant physical consequences when dislocations move at high speeds. For instance, in developing a 3D methodology of discrete dislocation dynamics (see [268]), Zbib and coworkers [269] only considered dislocation speeds to affect their mobility, where they were included via the inertial dislocation mass term developed by Hirth, Zbib and Lothe[265] (see section 5). Similar treatments were given by Wang and coworkers[270, 271, 272]: the sole high speed effect they considered was the 'inertia' affecting the equation of motion of dislocations, whilst the fields of the dislocations themselves were treated elastostatically.

This 3D methodology was used by Shehadeh and coworkers[237, 273] to study shock loading in copper, where they found that due to the strong increase in the dislocation density only about 1% of the dislocations were gliding at speeds higher than $\approx 0.8c_t$, with the vast majority moving at speeds well below $0.2c_t$. Unsurprisingly, this led Kubin to conclude that '*this relativistic regime seems to be rather unimportant*'([267],p.209). Most other observations, including the formation of microbands[274, 275] could be attributed to the large strain rates and stresses associated with the loading, rather than to any inherently 'relativistic' effect[267].

Similar conclusions regarding the 'relativistic' effect were reached in what paradoxically amounts to a far more sophisticated account of dislocation plasticity, namely that provided Roos et al.[277, 276]. Adapting in this case the plane strain dislocation dynamics formalism developed by Needleman and Van der Giessen[278], Roos et al.[277, 276] accounted not only for high speed effects in the mobility law, but also in the elastic fields of the dislocations themselves, which they modified to take the form of the uniformly moving edge dislocation's derived by Eshelby[11]. As is reproduced in fig.8, the study found that the main contribution to the global response was the inertia-like term that is postulated to affect high speed dislocation motion (see section 5) and entails a finite acceleration time: in comparing the elastostatic treatment to the dynamic treatment, the fields themselves appeared to lead to a statistically insignificant differences in the macroscopic response (see fig.8). The most important effect was not due to the dynamic fields of high speed dislocations, but to the finite acceleration time that dislocation inertia introduced into the model[276].

Gurrutxaga-Lerma et al.[222] brought to light further high speed effects affecting the plastic response of materials. In [222], they modelled the plastic relaxation of shock waves using planar dislocation dynamics[278]. In this, they followed Shehadeh and coworkers[273, 237], using the Needleman and Van der Giessen[278] dislocation dynamics approach in plane strain, which is based on elastostatics. They observed that this treatment invariably violated causality. In these simulations (reproduced in fig.9), they showed that, due to the vast numbers of dislocations generated behind the shock front, the instantaneous propagation of their elastostatic fields throughout the entire system activated dislocation sources ahead of the shock front, in direct contravention of causality. As the simulation progressed, the spurious nucleation of dislocations ahead of the shock front became just as strong as the generation behind the front.

The material ahead of the shock front is unaware of it until the shock front reaches it. Only then should dislocations be nucleated. This is the meaning of causality in the context of the plastic relaxation of an elastic shock wave. The violation of causality turned out to be the major feature of the elastodynamic dislocation that had been overlooked

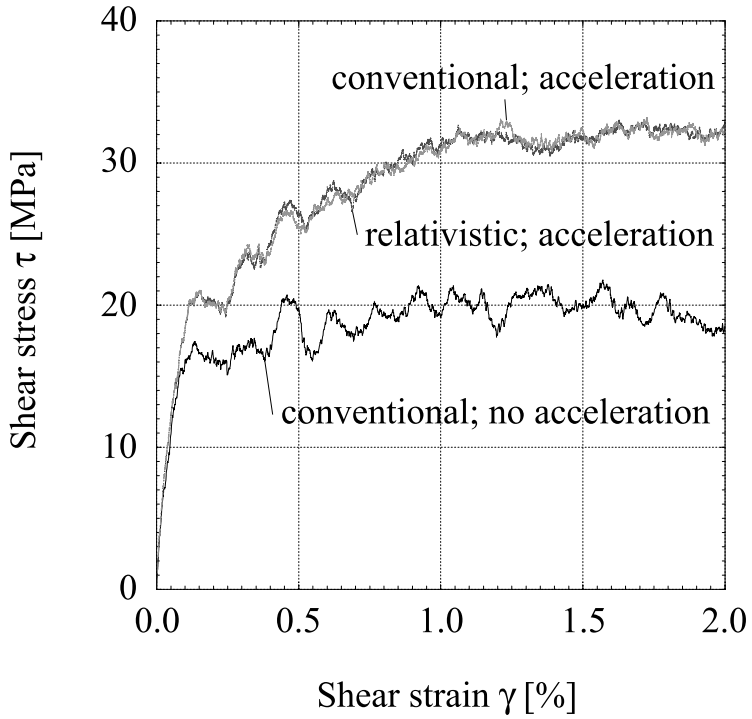


Figure 8: The Stress-strain curve of the quasi-dynamic dislocation dynamic simulations performed by Roos et al.[276]. A strip of Cu was loaded at $10^6 s^{-1}$ and 100K, and the stress hardening response under three conditions was compared: conventional dislocation plasticity, with no inertia effects; 'accelerated' conventional dislocation plasticity, with a mobility law containing a dislocation mass and inertia term; 'relativistic' dislocation plasticity, which includes both a high speed mobility law and the dynamic fields of a uniformly moving dislocation derived by Eshelby[190]. This article was published in Computational Materials Science, 20, Roos et al., A two-dimensional computational methodology for high-speed dislocations in high strain-rate deformation, 1–18, Copyright Elsevier (2001).

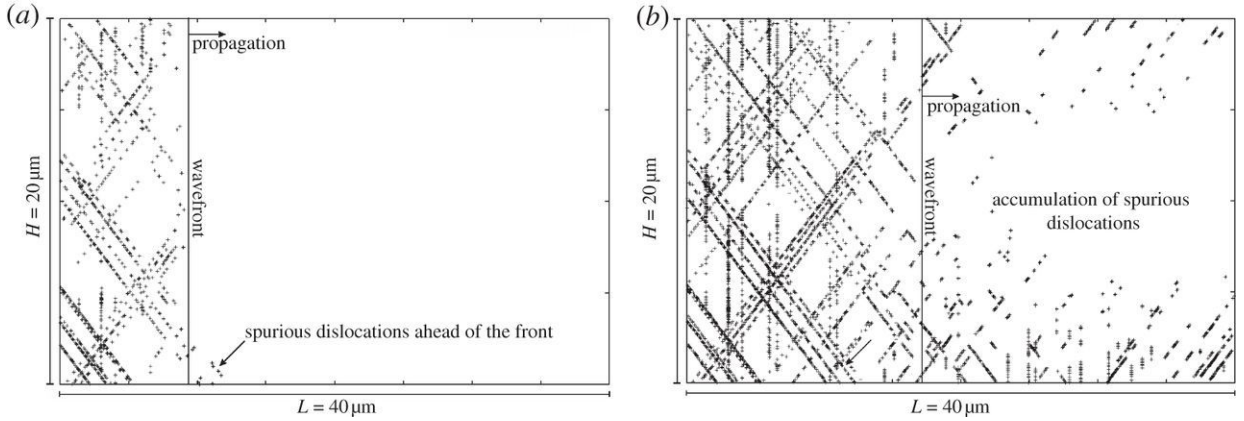


Figure 9: The elastodynamic treatment of dislocations becomes necessary when the external stimulus triggering dislocation activity (in the figure, a shock front depicted at two different instants in (a) and (b)) propagates at speeds close to the speed of sound. In that case, an elastostatic account will invariably violate causality, and trigger factitious effect such as the spurious nucleation of dislocations reported in this figure by Gurrutxaga-Lerma et al.[222]. Reproduced from Gurrutxaga-Lerma et al.[222] under CC BY 4.0.

hitherto, an effect that the treatment offered by Shehadeh et al.[237], Wang et al.[270] and Roos et al.[277, 276] failed to capture because they used static or steady state dynamic solutions, which do not propagate.

The only way to avoid it would be to offer a fully elastodynamic account of the non-uniform motion of dislocations, which Gurrutxaga-Lerma et al.[222] were the first to do. They used Markenscoff and Clifton's, elastodynamic solution for a non-uniformly moving edge dislocation[217], which they augmented with their own derivation of the elastodynamic field accompanying the instantaneous creation of an edge dislocation. The result is a method of considerable computational complexity, which these authors employed to study the attenuation of the dynamic yield point[238], and the shielding of dynamic cracks[232]. Recently, Cui and coworkers [279] started extend this treatment to 3D dislocations, using the formalism developed by Mura[185] in eqn.19 for closed loops.

The picture of plasticity that arises from an elastodynamic treatment of dislocation plasticity is very different from the static treatments in textbooks. Dislocations interact with one another based on a retardation principle[222], so that it takes a finite time for the elastic fields to travel from one point to another. Furthermore, the elastic field of a dislocation now depends not only on its current location but on all its previous locations, as illustrated in fig.9. A dislocation responds to the presence of a second dislocation only when sufficient time has passed for the field of the second dislocation to reach it, in accordance with causality. The interactions are asymmetric: unlike the steady-state and elastostatic solutions[1], Doppler-like magnifications appear ahead of the dislocation core, but not behind. Such effects appear crucial in explaining the relaxation of a shock front[238], even though the dislocations generated at the shock front travel at speeds well below c_t. Screw and edge dislocations interact at different fundamental speeds: the field of screw dislocations propagates at the transverse speed of sound, whilst that of edge dislocations travels at both the longitudinal and transverse speeds. Thus for instance, plastic activity in a shock front travelling at the longitudinal speed of sound cannot be influenced by the screw components.

A dichotomy arises between the elastodynamic field of a moving dislocation and its equation of motion. Whereas the former is captured by the theory of elastodynamics with refinements such as regularisation of the core, the latter involves a host of additional physics that is absent in elastodynamics, and which arises from the movement of the dislocation through a dynamical crystal lattice, not through a continuum (see section 5).

3.5 The effect of anisotropy

High speed dislocations in anisotropic linear elastic media have received less attention than their isotropic counterparts. Nevertheless, the main characteristics of the linear elastic anisotropic problem remain largely the same: there are limiting velocities that correspond to the three speeds of sound, which in general depend on the direction of propagation within the crystal. As in the isotropic case, the (generalised) Rayleigh wave speed may also play a role in reversing the sign of the interactions between like-signed dislocations. Solutions to the uniformly moving 'steady state' problem were achieved by by Sáenz [280] and Bullough and Bilby [281]. The main features of the solutions for the screw dislocation suggest that a singularity exists at the shear wave speed, in this case given by

$$c_\infty = \sqrt{\frac{C_{44}C_{55} - C_{45}^2}{\rho C_{44}}} \tag{20}$$

where C_{44}, C_{45} and C_{55} are the elastic constants using the standard Voigt notation[282], and ρ the density. This corresponds to the first transverse wave speed under antiplanar conditions (see [282, 283]).

This suggests that, in contrast with the isotropic case, the crystallographic orientation of the glide plane plays a crucial role in the critical velocities of dislocation motion. This topic was examined in detail by Teutonico[284, 285, 286], who first provided expressions for the elastic self-energy of the uniformly moving edge and screw dislocations in anisotropic media[284] and for the displacement fields of the motion along arbitrary orientations[286]. Crucially, Teutonico found that as in the isotropic case, anisotropic linear elasticity predicted limiting velocities at c_∞ for screw dislocations. For edge dislocations however, the limiting velocity would generally be the of the form[284]

$$c_1 = \sqrt{\frac{C_{66}}{\rho}} \tag{21}$$

Depending on the orientation, it is possible for C_{66} to be different from the largest C_{66}, i.e., for the limiting speed c_1 of an edge dislocation in anisotropic media to be smaller than the corresponding transverse speed of sound[284].

Furthermore, in analogy to the Rayleigh wave instabilities we discussed in section 3.3, Teutonico [284, 286] examined the presence of analogous '*threshold*' velocities above which the sign of the shear stress field along the slip plane would reverse. As in the isotropic case, he found no such threshold speed for screw dislocations, whereas for edge dislocations he found that depending on orientation, the threshold velocity could be any between 0 and c_1.

Work by Weertman[287, 288] and collaborators [289] and by Teutonico[290] focused on performing similar analyses for specific crystalline structures and orientations, similarly finding the values of the limiting and threshold velocities for the steady state motion.

The steady state problem of a moving dislocation in an anisotropic medium was given a complete treatment by Stroh[27], who using the approach he had originally developed for static dislocations in [291], examined both the energetics and the general expression for the displacement fields and at the same time developed what is nowadays known as the '*Stroh formalism*', a powerful method for the analysis of particular solutions in anisotropic elasticity (see [282, 283, 292, 293]). The results derived by Stroh for the uniformly moving anisotropic dislocation were used by Barnett and Lothe [294, 295, 296] to examine the question of the existence and uniqueness of free surface waves in anisotropic media.

Beltz et al.[297] generalised Lothe's[298] and Brown's[299] formulae for the self-force on a curved dislocation segment to the steady state solution of the uniformly moving arbitrary dislocation. Similarly, using the approach originally developed by Willis[300] to obtain the elastic field of an arbitrary dislocation segment in an anisotropic medium, Mura[301] obtained the elastic field for the steady state motion of an arbitrary segment.

In turn, the transient solutions were fully achieved by Markenscoff and Ni for screw [302] and edge dislocations under cubic and hexagonal symmetry[303, 304], and further generalised to arbitrary motions and general anisotropy by these same authors [305]. The transient solutions also display the characteristic limiting speeds associated with the steady state, which in elastic anisotropy these are not constant — they depend on the direction of propagation. However, as in the isotropic case, the solutions describe the dislocations as wave sources, in this case radiated at the characteristic speeds of sound of the medium, which are governed by its anisotropy. Thus, the energy released and the elastic field profiles can be considerably different, and may display cusp-like wave fronts[305].

4 Atomistic models of gliding dislocation

Although the transient elastodynamic models reviewed in section 3.3 provide an accurate long range description of the mechanical interactions between dislocations and other defects, the singularities at the cores of Volterra dislocations and at the speeds of sound, and their lack of dispersive mechanisms (i.e., drag) suggest that linear elastic models fail to recognise that dislocations are in a crystal lattice with sufficient accuracy.

Atomistic studies of high speed dislocations can be used to address three elements missed in linear elasticity: the discreteness of crystalline materials, the coupling between dislocations and crystal lattice vibrations, and the anharmonicity of interatomic forces. The crystal lattice introduces a length scale absent in continuum models, namely the smallest separation of atoms. This is the minimum width of a dislocation core and its finiteness removes singularities in the elastic field of the dislocation. The dislocation is coupled to the crystal lattice. As it glides it excites crystal lattice vibrations, like running a finger along the keyboard of a piano. The radiation of vibrations is the principal reason why dislocation motion is overdamped. In stark contrast to the FE continuum model of a dislocation gliding at a constant speed, where no force is required to maintain its constant speed, in a crystal lattices it is stopped within a few lattice vibration periods once the glide force on it is removed. The stiffnesses of bonds in the core depart significantly from those in the bulk owing to the anharmonicity of atomic interactions. This keeps the stresses generated in the core finite even though the strains may be very large, and it also affects the scattering of crystal lattice vibrations arriving at the core, which also contributes to the drag on the dislocation.

4.1 Lattice dynamics models

The first atomic scale models of uniformly moving dislocations were lattice dynamics models. These describe the reaction of a crystalline lattice, treated within the harmonic approximation, to a prescribed driving force [306, 307]. They therefore serve to capture discreteness effects, but not anharmonicities. Lattice dynamics models first emerged in atomic scale investigations of point defects [308, 309, 310], and the method was successfully extended to treat dislocations [311, 312, 313].

The oldest lattice dynamics studies of gliding dislocations were a family of related models called *snapping bond models* [314, 23, 24]. These generated the required dislocation displacement jump, with magnitude equal to the Burgers vector, by explicitly breaking and restoring atomic bonds across the glide plane [314, 23, 24, 241, 315, 25] – hence the name. However, these were often simple models of Frenkel-Kontorova (FK) [174] type or of gliding dislocations in square or simple cubic lattices. They allowed the dislocation–lattice interactions to be investigated directly [316, 317]. Furthermore, they allowed two atomistic drag mechanisms to be studied separately. A gliding dislocation suffers drag from the scattering of pre-existing crystal lattice vibrations [318], a phenomenon referred to as *phonon wind*. On the other hand, a dislocation generates lattice wave radiation as it glides through the lattice [314, 23, 24, 315, 25]. Together,

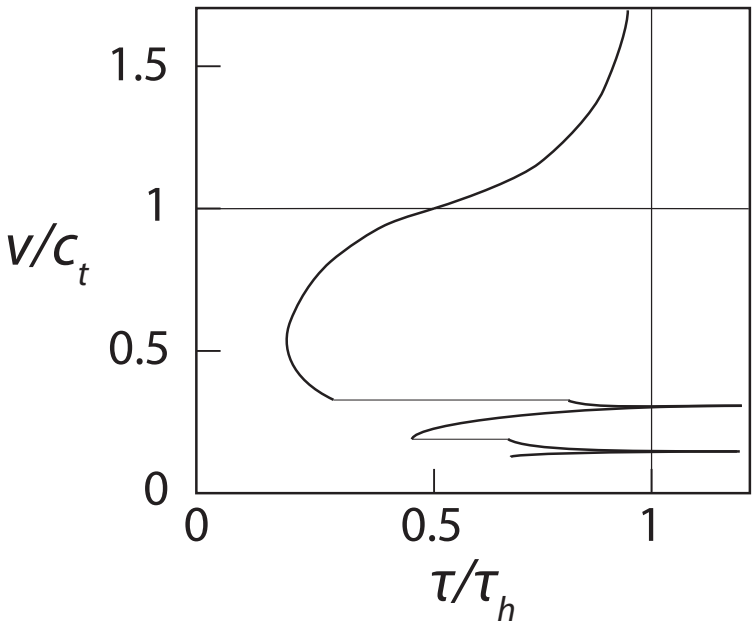


Figure 10: The speed v of the dislocation, normalised to the shear wave speed c_t, plotted against the resolved shear stress τ, normalised to the ideal lattice strength τ_h, for uniformly moving screw dislocation in a simple cubic lattice dynamics model with nearest neighbour interactions. The continuity jumps at low speeds denote fundamental instabilities. Adapted from Ishioka [24].

these two effects constitute the *phonon drag* that eluded contemporary continuum models. Moreover, being able to quantify these energy dissipation mechanisms also allowed the explicit derivation of precise relationships between the dislocation's velocity and the force required to maintain uniform motion. A representative example of such a *mobility law* derived from a lattice dynamics model of a uniformly moving screw dislocation in a square lattice is shown in fig.10 [24].

As shown in fig.10, in lattice dynamics models nothing of note occurs at the shear wave speed. As far as lattice models were concerned, this was the end of the discussion as all related works were in complete agreement on this [314, 23, 24, 241, 315, 25]. This suggested that the shear wave speed is given a particular status within elastodynamic continuum models of gliding dislocations (cf. section 3) due to the highly simplified dispersion relations ($\omega = c(\hat{k})k$) they subsume [313]: Dispersion in the phonon spectrum invariably facilitates the avoidance of singularities encountered in elastodynamics at the speeds of sound.

Lattice dynamic models display a second feature visible in fig.10: at velocities below approximately $c_t/3$, these models contained clear instabilities. These were investigated in great mathematical detail by Rogula [319, 320, 321]. They were found to occur at dislocation velocities where both phase and group velocities of the excited lattice vibrations were equal to the dislocation's velocity. If such state was reached, the dislocation core is unable to evacuate energy in any spatial direction, and the atoms at either side of the dislocation core enter resonance.

It is instructive to investigate the occurrences of these resonances in greater detail as this also reveals why supersonic dislocations are a possible in harmonic lattice models. The governing equation of a harmonic lattice model is the classical linear momentum conservation, with a viscosity term(cf. [310]):

$$M\frac{\partial^2 u_{i\alpha}(t)}{\partial t^2} = -D_{i\alpha,j\beta}u_{j\beta}(t) - 2M\Gamma\frac{\partial u_{i\alpha}(t)}{\partial t} \tag{22}$$

where $u_{i\alpha}$ is the α^{th} component of the displacement of atom i, which are defined as the difference between the current position $r_{i\alpha}$ and the perfect lattice position $R_{i\alpha}$ of the atom α: $u_{i\alpha} = r_{i\alpha} - R_{i\alpha}$. Equally, M is the mass of the atoms in the lattice, and

$$D_{i\alpha,j\beta} = D_{\alpha\beta}(\mathbf{r}_i, \mathbf{r}_j) = \left.\frac{\partial^2 U}{\partial r_{i\alpha} r_{j\beta}}\right|_{\{\mathbf{R}_i^0\}}$$

is the *force constant matrix* of the harmonic lattice, measuring the interatomic forces, for $\mathbf{r}_i$ the lattice position of atom i relative to the perfect lattice positions $\mathbf{R}_i^0$. The parameter Γ is the strength of a viscous damping term, included to

reduce the heating: physically it may be thought of as a means of capturing the energy transfer to degrees of freedom excluded in the harmonic lattice model, such as electrons.

As eqn.22 is linear, its solution may be expressed in terms of the lattice Green's function as follows[310]:

$$\mathbf{u}(\mathbf{r}_i, t) = \sum_j \int_{-\infty}^{\infty} \mathrm{d}t' \mathbf{G}(\mathbf{r}_i - \mathbf{r}_j, t - t') \mathbf{f}_K(\mathbf{r}_j, t') \tag{23}$$

where $\mathbf{f}_K(\mathbf{r}_j, t')$ is any source term expressed as a Kanzaki force distribution[309, 313, 322]. By source term we mean any boundary condition; because equation 22 is a force balance, we require the boundary condition to be expressed as a distribution of forces acting on the atoms of the perfect lattice. In this case, these forces would have to be those that when acting on the atoms of the perfect lattice generate the displacement field of a dislocation. This makes the forces be *Kanzaki forces*[309, 25, 313, 322]. In the case of a uniformly gliding screw dislocation, the Kanzaki force distribution that acts as a source term is given by[25, 313]

$$\mathbf{f}_K(\mathbf{r}_j, t) = \sum_{\beta,j} B\delta_{z\beta}\Psi_{ij} D_{i\alpha j\beta} \mathrm{H}(vt - x_i) \tag{24}$$

where $\Psi_{ij} = \pm 1$ if the particle i is above (below) the glide plane and j below (above), and 0 otherwise. Here, the Kanzaki forces arise as force doublets (see [313]) acting on either side of the slip plane. This is because atoms on either side of the slip plane experience equal and opposite forces that bring about the Burgers vector-sized relative displacement across the slip plane. The gliding dislocation is thus a distribution of Kanzaki force dipoles moving along the slip plane, the effect of which is to expand the region that has undergone the relative displacement across the slip plane by the Burgers vector. This is what happens in the core of a gliding dislocation.

Eqn.22, is first expressed in Fourier space, where the convolution becomes a product. In Fourier space, the Green's function takes the form [323]

$$\tilde{\mathbf{G}}_{\alpha\beta}(\mathbf{k}, \omega) = \frac{1}{M} \sum_b \frac{\tilde{u}_\alpha(\mathbf{k}, b)\tilde{u}^*_\beta(\mathbf{k}, b)}{\omega^2(\mathbf{k}, b) - \omega^2 + 2i\Gamma\omega} \tag{25}$$

where $\omega(\mathbf{k}, b)$ is the lattice wave dispersion relation, b the branch index, ~denotes a variable in Fourier space and $*$ indicates complex conjugation.

The inversion along the glissile direction leads to

$$u_z(x_i, t) = -\frac{4B}{k_y^b \pi M} \sum_{l>0,b,\beta} \int_0^{k_y^b} \mathrm{d}k_y \int_0^{\infty} \mathrm{d}k_x F_{\beta l} \sin(k_y y_j) \sin(k_y y_1) \tilde{u}_z(\mathbf{k}, b) \tilde{u}^*_\beta(\mathbf{k}, b) \times$$
$$\times \left\{ \frac{\left(\omega^2(\mathbf{k}, b) - v^2 k_x^2\right) \sin\left[k_x(x_i - vt)\right] + 2\Gamma v k_x \cos\left[k_x(x_i - vt)\right]}{(k_x + i\epsilon)\left[(\omega^2(\mathbf{k}, b) - v^2 k_x^2)^2 + 4\Gamma^2 v^2 k_x^2\right]} - \frac{\pi\delta(k_x)}{2\omega^2(\mathbf{k}, b)} \right\} \tag{26}$$

where k_x, k_y are the components of the Fourier space $\mathbf{k}$ vector, k_y^b is the maximum value of k_y found in the lattice's Brillouin zone[159].

In principle, the displacement field u_z diverges if $\omega(\mathbf{k}, b) = vk_x$ and $k_x \neq 0$. Note that if $k_x = 0$ the numerator does not diverge, so $k_x \neq 0$ is also a necessary condition of resonance.

However, this is not a sufficient criterion for resonance. As studied at different levels of refinement by Rogula [319, 320, 321], Atkinson and Cabrera[314], Ishioka[26], and Celli and Flytzanis[23], an additional requirement for resonance is that the energy associated with the moving dislocation (not reproduced here) diverges at the same time as the displacement field in eqn.26 does.

The dislocation's energy in the harmonic lattice diverges only if the dislocation speed is equal to the group velocity of the lattice[319, 320, 321]. In that case, the energy radiated by the dislocation cannot escape the dislocation core, and a strong resonance is triggered.

Thus, whereas linear elasticity predicts singularities when $v = c_t$, harmonic lattice models predict singularities when the speed of a screw dislocation satisfies

$$\underbrace{\frac{\partial\omega(\mathbf{k})}{\partial k_x}}_{v_{\text{group}}} = \underbrace{\frac{\omega(\mathbf{k})}{k_x}}_{v_{\text{phase}}} = v \tag{27}$$

The speeds at which this condition is met are called *breakdown velocities*[25].

Eqn. 27 helps understand why linear elasticity predicts divergences at the speed of sound. Let us assume a simple 'elastic' lattice: the dispersion relation in linear elasticity is $\omega = c_i k$ where $c_i = c_t$ or $c_i = c_l$. This means that linear elastic media are non-dispersive (cf.[324]). In linear elasticity the resonance condition (eqn.27) is met when

$$v = \frac{c_i k}{k} = \frac{\partial (c_i k)}{\partial k} = c_i \tag{28}$$

irrespective of the wavenumber. Thus, in a linear elastic medium, the speed of sound is the only possible breakdown velocity.

However, this condition is not met in real dispersive lattices. This is due to the convexity of the dispersion relation, and the requirement that $k_x \neq 0$. In particular, for a realistic dispersion relation in a crystal, the only wavenumber for which the group velocity $\frac{\partial \omega(\mathbf{k})}{\partial k_x}$ is the speed of sound (c_t or c_l) is $k_x = 0$. However, this violates the necessary condition that $k_x = 0$ for a resonance to be triggered in eqn.26.

Hence, in a real crystal the resonance condition cannot be met at the speeds of sound. Thus, harmonic lattice models predict that 'nothing special' will happen at the speeds of sound[159]. However, harmonic lattice models do contain divergences at the resonant 'breakdown velocities', which in realistic models of a crystal tend to happen at relatively high wavenumbers[324], i.e., at moderate and low dislocation glide speeds, and are heavily dependent on the material's specific dispersion relation $\omega(\mathbf{k})$.

These 'breakdown' resonances were problematic because they implied that for dislocations travelling at speeds below approximately $c_t/3$, their displacement field should diverge or at least contain regions with very large displacements. This contradicts the small displacement assumption [314], in the form of the harmonic approximation, at the heart of lattice models [50]. This sparked some high-profile criticism, most notably in Alshits [50] and Hirth and Lothe [1] (p. 208), the fact notwithstanding that the alternative, linear elasticity, is in fact a limiting case of the harmonic lattice[307].

These criticism weighted heavy on lattice models that were already becoming unfashionable due to their apparent simplicity[50]. The simple cubic systems under consideration raised the question whether these models were at all representative of dislocations propagating in real crystals. In particular, it was questioned whether many of the unexpected results were not the result of the simplified lattice structures[325], whether the harmonic interatomic interactions in these early lattice models were justified [26, 241, 326, 327] and whether the assumed uniform motion was internally consistent within them [26, 328, 329, 242, 155, 50]. Additional problems may be found in these highly simplified model of the dislocation. For instance, eqn.24 is the typical distribution of forces employed in lattice models to model gliding screw dislocation. The core is just one bond length wide, and is assumed to remain the same irrespective of the glide speed. This may be true when the core is spread in the slip plane, but fails to account for the non-planar core in BCC metals[330], and assumes translational symmetry along the dislocation line, which omits treating the kink mechanism of dislocation movement. Although some of the resonances entailed by eqn.27 appear to be independent of the core structure itself [159], it is likely that some at least be cancelled, as is the case in elastodynamics.

In most cases, these limitations are an inevitable consequence of the desire to keep the models analytically soluble. Using computer simulations of harmonic lattice models, it was argued that at velocities just below c_t, uniform dislocation motion seemed no longer possible [328, 242, 331] owing to the presence of further breakdown phenomena when the dislocation speed reached $0.9 - 9.99c_t$. In addition, it was suggested that these *breakdown velocities* could be critical or bifurcation points, and provide onset mechanisms for kinematic generation and twinning [242, 241]. In particular [155, 325, 332, 331, 159], it has been suggested[155, 325, 159] that they provide a rationale for the kinematic generation mechanism that Weertman[168] had associated with the Rayleigh wave speed in linear elasticity. In fact, despite seemingly rejecting harmonic lattice models, Hirth and Lothe[1] used the results in [155] to support their view that kinematic generation of dislocations exists.

These studies brought the existential question of supersonic dislocations to the fore once more, though for reasons very different from the inertial arguments presented by continuum theories [328]. Fundamentally, they suggested that supersonic motion was largely possible due to the discreteness in the lattice, rather than a consequence of non-linear elastic effects. However, the occurrence of breakdown speeds was considered implausible, and harmonic lattice models fell out of favour. The continuum perspective, whereby dislocations are able to glide impeded only by vibrational and electronic excitations up to around $c_t/2$ beyond which inertial effects were thought to dominate, remained the consensus[1].

4.2 Molecular dynamics simulations

Lattice models were succeeded by the advent of the molecular dynamics (MD) simulations [333] as the required computing power to simulate adequately sized systems with more realistic interatomic potentialsatomic interaction potentials for metals [334, 335, 336, 337] became available, particularly starting in the mid 1990s.

MD simulations possess the same same advantages as the lattice dynamics models compared to continuum models: it allows detailed investigations of the dislocation–lattice interaction, although it remains a classical (non-quantised) description of that interaction. Unlike harmonic lattice models, no assumptions are made about the structure of the dislocation core, either when it is stationary or moving. The core does not have to be planar, and in some important cases it is three dimensional[338, 330]. The dislocation does not have to move *en masse* maintaining translational symmetry along the line, and it can move by a kink mechanism (see [1]).

Despite these improvements there are still significant limitations in MD simulations of any crystal defect. Although the interatomic potentials avoid the harmonic approximation, they are still far from a solution of the many body quantum mechanical problem of how atoms interact in solids. The vast majority of interatomic potentials have been empirically constructed by fitting an assumed functional form to experimental data or data derived from density functional calculations[339]. The atomic equations of motion in an MD simulation are Newtonian and hence the atomic dynamics is classical[333]. This means that the interaction with, and generation of, lattice vibrations is unreliable at temperatures below the Debye temperature where quantum statistics dominates. Finally, there are always concerns about the system size and boundary conditions applied to the computational cell. Whereas in the harmonic lattice model the gliding dislocation is modelled in an infinite crystal lattice, in an MD simulation it is either in a crystallite with free surfaces or a large cell that is repeated periodically. The presence of free surfaces or periodic boundaries can influence the simulation if the dislocation becomes aware of their presence through reflected waves or spurious interactions with itself through periodic boundaries.

It was the seminal 1999 paper by Gumbsch and Gao [157] in particular which provided the spark that inspired a flurry of subsequent MD studies of fast moving dislocations [340, 341, 342, 343, 344, 237, 345, 346, 272, 347, 348, 349, 350, 351, 352]. Although in 1995 Schiøtz et al.[156] had already reported the presence of transonic dislocations in MD simulations of kinematic generation, this was the first MD simulation that focused on the existence of supersonic dislocations [157] as shown in fig.11. Gumbsch and Gao's results were in perfect agreement with the results offered by older harmonic lattice models, and were subsequently confirmed in further MD simulations of dislocations in other materials [340, 346, 347, 348, 350, 351]. Hitherto, it was widely accepted that the speed of sound was indeed a hard barrier for dislocation motion, as the main counterarguments came from lattice dynamics models that were perceived to be unreliable (cf. section 4.1). Hence, it is not surprising that this first observation of supersonic edge dislocations in computer experiments caused a stir in the field. So much so that it also revitalised the interest in the topic within the continuum elastodynamics community, inspiring some of the post-1999 elastodynamic studies reviewed in sections 3.3, aimed at explaining this discrepancy.

The second driver behind MD studies of high speed dislocations was the need for dislocation mobility laws in the pure glide regime [353, 354]. As explained in the *Introduction*, this mobility law is one of the main quantities through which this atomistic - continuum divide is bridged. In the absence of experimental measurements, an obvious strategy to obtain such a relation is to perform MD simulations of gliding dislocations from which a quantitative velocity-stress relation to be used in DD simulations may be obtained [235, 355, 158, 346, 351, 352, 356, 345, 357, 358, 359]. Associated instabilities affecting high speed dislocations concerning dislocation interactions at high speed have also been explored [360, 361]. Figure 12 shows a typical result from these simulations: as the applied stress level is increased, the steady state speed achieved in this case by an edge dislocation in fcc Al tends to saturate towards c_t[351, 158], but does not prevent transonic motion, which may display instabilities or 'jumps'[158, 157]. Comparable MD simulations of screw dislocations[158] suggest that this saturation plateau below c_t may be narrower or non-existent for, easing the transonic transition of screw dislocations. These findings reinforce the view that inertial effects condition the transition between subsonic and transonic dislocations.

Finally, a third group of MD dislocation dynamics studies exist with the aim to understand the physics of the dislocation–lattice interaction [325, 343, 345, 362, 363]. However, despite the physical richness inherent to modern MD simulations it proved difficult to extract transferable, generally applicable, qualitative results from these [343, 345, 362]. So much so that some took a step back and performed much simpler MD simulations, reminiscent of the lattice models discussed in section 4.1 [325, 342]. The most notable result coming out of these studies was the observation of kinematic generation of screw dislocations in square and hexagonal lattices, a process that can not be accounted for within linear elasticity [325]. The kinematic generation of edge dislocations, allowed in elastic continuum theories as discussed in section 3.3.3, had been confirmed in MD simulations by Schiøtz et al.[156]. In [159] (see fig.13), it was shown that in MD simulations of screw dislocations in bcc W, kinematic generation occurred at the breakdown velocities predicted by equivalent harmonic lattice calculations ($\approx 0.24c_t$). Shock loading and other high strain rate processes can also be explored using MD simulations; Hahn et al.[234] (see fig.14), Ruestes et al.[350] and others (see for instance [236, 364, 365, 366]) have used this method to explore the role dislocation generation and high speed motion play in relaxing a shock front.

Thus, MD simulations of increasing complexity and harmonic lattice models suggest that the sound barrier is not insurmountable. Furthermore, a subset of the MD simulations also display instabilities in gliding dislocations may

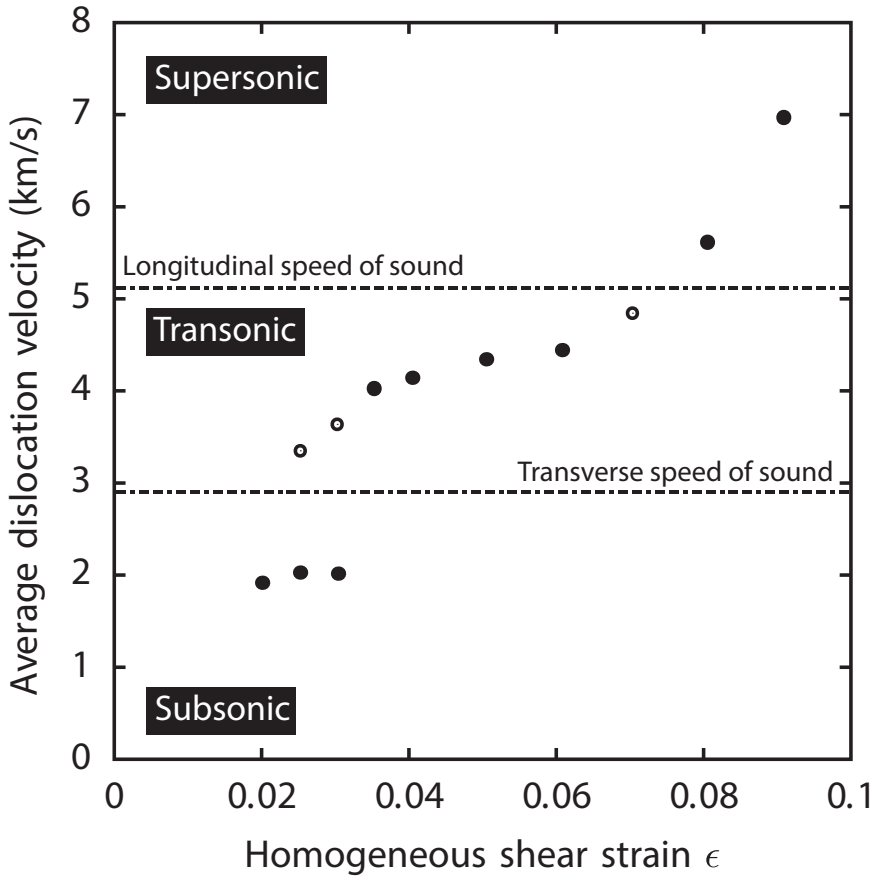


Figure 11: Observed average dislocation velocity for edge dislocations in MD simulations of tungsten [335, 336]. Solid circles indicate stable dislocation motion whereas open circles mark the average velocities at which the observed motion was unstable and varied significantly throughout the simulation. Figure adapted from Gumbsch and Gao[157].

trigger a kinematic generation mechanism. The fact that both harmonic lattice models and MD simulations display both features suggests that these effects are mediated more by the discreteness of the lattice rather than by anharmonicities. This situation is reminiscent of the *lattice trapping* effect thought to control the propagation of brittle cracks, as opposed to other non-linearities owing to the extremely high stresses expected the crack tip [367, 368, 369, 370]. It also gives credibility to the existence of other associated instabilities, such as the kinematic generation of twins [371, 372], and that the physical cause of the 'debris' observed behind fast moving screw dislocations in MD simulations [373] is found in intrinsic instabilities of the dislocation line. Furthermore, because the lattice models fail to model the core as anything other than atomic-thin layer[25, 159] yet they display these same two features observed in MD simulations, it would appear that the role played by the dislocation core in facilitating supersonic motion or leading to instabilities is secondary. This does not mean that the core is irrelevant. To the contrary, the energy radiated by the dislocation, which manifests itself as a drag force, the energetics of dislocation glide and some of the instabilities observed (particularly in edge dislocations with wide stacking faults, cf.[346, 348]) are all expected to be dependent on the core structure.

In many ways it is challenging to understand why MD simulations have not been able to resolve the outstanding issues left by continuum theories. Today's computational resources allow the simulation of systems containing hundreds of millions of atoms [374] with interaction potentials with near density functional theory level accuracy that describe dislocation core structures with assumed reliability [337, 375, 376]. Yet nowadays, we still do not talk about *the* mobility law for a given dislocation topology in a material [354]. This is because so far an unequivocal picture of the phenomenology of gliding dislocations has not emerged from the multitude of MD studies that have been undertaken ([340, 341, 342, 343, 344, 237, 345, 346, 272, 347, 348, 349, 350, 351, 352] i. a.). Assuming that the vast majority of the MD simulations in the literature have been performed correctly, it is not at all obvious why this is the case.

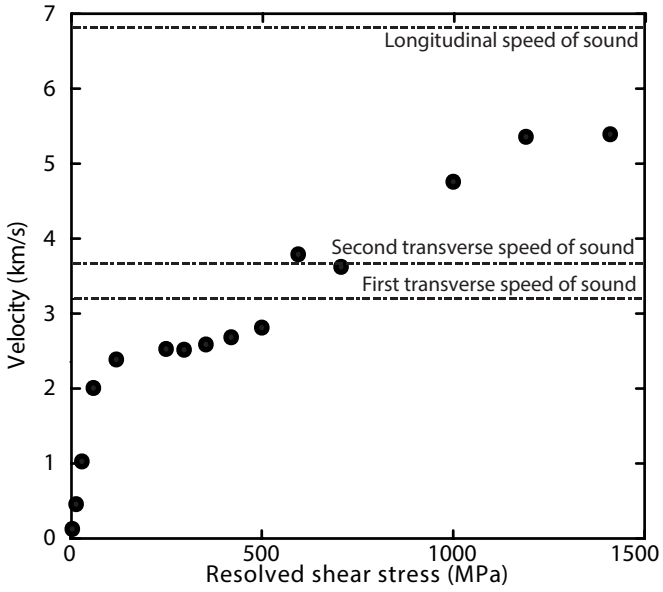


Figure 12: The stress-velocity curve of an edge dislocation in fcc Al at 216K, as observed in MD simulations by Olmsted et al.[158] The linear 'viscous drag' regime is observed at low stress levels; dislocation speed then appears to saturate as the dislocation approaches the first transverse speed of sound (about 3100m/s), which the simulation shows is overcome at least to the transonic regime. Data adapted from Olmsted et al.[158].

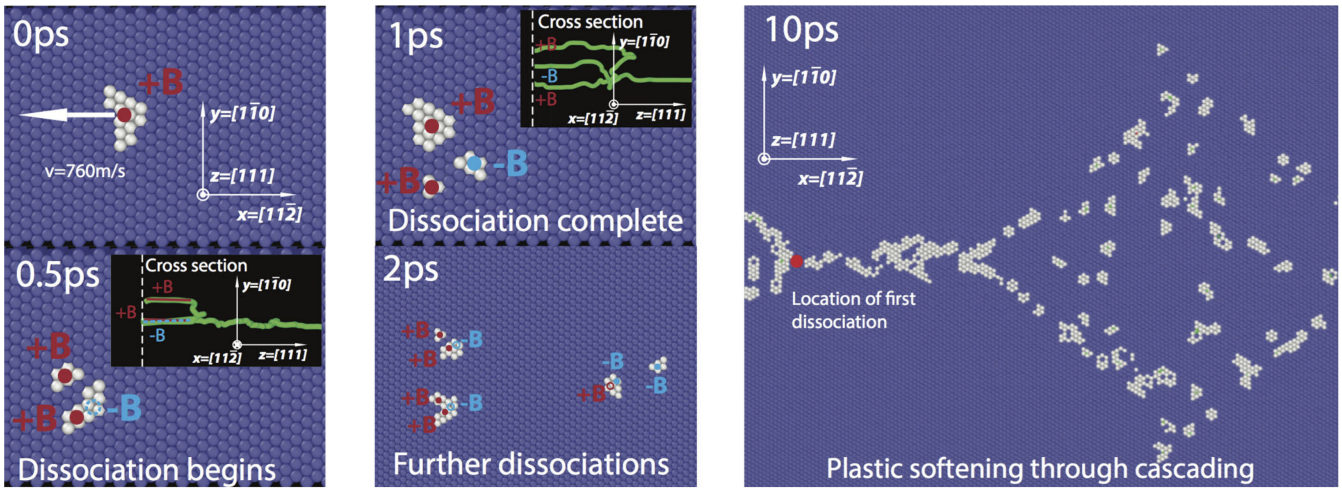


Figure 13: MD simulation of a screw dislocation gliding at 760m/s showcases the presence of fundamental lattice instabilities that lead to the dissociation of the dislocation via kinematic generation. Figure reproduced from Verschueren et al.[159] under CC BY 4.0.

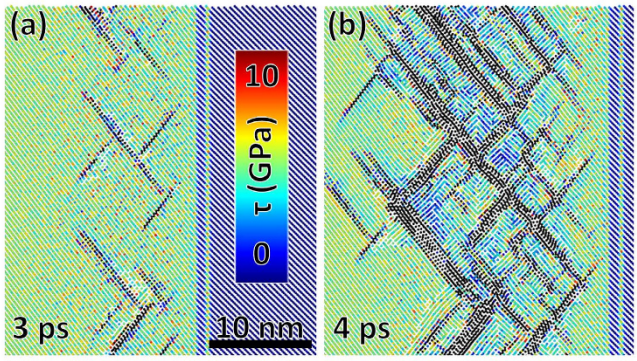


Figure 14: Homogeneously nucleated dislocations in an MD simulation of shock-loaded Si at $\tau = 6.4$GPa, performed by Hahn et al.[234]. The dislocations thus nucleated were reported to achieve speeds in excess of 13km/s, and lead within 4ps to significant plastic relaxation of the Si crystallite (shown in fig.b). Figure reproduced from Hahn et al.[234] under CC BY 4.0.

5 Dislocation Mobility

The aim of most of the work we have reviewed is to achieve physical description of the mobility of high speed dislocations. Dislocations move so as to minimise the potential energy of the material and any external loading mechanism[187, 1]. In so doing, they experience a conservative force known as the *Peach-Koehler (PK) force*[37], independent of the mathematical description of the dislocation itself. The energy released in moving is dissipated by the lattice through a number of damping and attenuation mechanisms that manifest themselves in the form of a *drag force*.

A *mobility law* typically expresses a force balance between the PK force and a drag force:

$$f_{\text{PK}} = f_{\text{drag}}(v, \dot{v}, \tau, T, \ldots)$$

In accounting for high speed effects, the mathematical form of both sides of the equation must be addressed. The PK force is subject to particular considerations under dynamic (time-dependent) loading. The drag force is primarily informed by theory and simulation owing to the lack of direct experimental observation of high speed dislocations. It may account for a number of physical mechanisms including *inertia* and *phonon drag*. These two terms are explained in the following.

Why dislocation mobility matters. The importance of the mobility law cannot be overstated. It is one of the crucial ingredients in dislocation plasticity, since the plastic response of materials is understood to be governed by slip mediated by dislocations[377, 267]. Its importance may be understood through Orowan's equation[39], which provides the average (cf.[378, 379]) macroscopic plastic strain rate $\dot{\gamma}_p$:

$$\dot{\gamma}_p = B\rho_d\bar{v} \tag{29}$$

where B is the Burgers vector's magnitude, ρ_d is the density of mobile dislocations, and $\bar{v}$ the average speed of the moving dislocations. Clearly, knowledge of $\bar{v}$ becomes crucial if a physically motivated expression of $\dot{\gamma}_p$ is to be found. The Orowan equation is the basis of many crystal plasticity models (see for instance [380, 381, 382]), where a mobility law involving $\bar{v}$ is usually embedded in some phenomenological way (see [383, 384, 385, 386, 387] for different applications).

Dislocation mobility is also needed in discrete dislocation dynamics simulations [388, 353]. In discrete dislocation dynamics simulations dislocation microstructures evolve through forces between dislocations calculated using elasticity theory. Short-range interactions such as dislocation reactions are handled through rules supplied by the user, the mobility law (along with dislocation generation[389]) being one.

5.1 The dynamic Peach-Koehler force

The PK force is a configurational force (cf.[390]), defined as the gradient of the Gibbs potential[391] or, equivalently, through the static energy-momentum tensor[187] on the dislocation. It takes the well-known form[37, 1]

$$f_n^{PK} = \epsilon_{njm}\sigma_{ij}B_i\xi_m \tag{30}$$

for a dislocation of Burgers vector B_i, line direction ξ_m, subjected to a external stress field σ_{ij}, and ϵ_{njm} the Levi-Civita symbol.

The validity of the PK force under dynamic conditions is not obvious. The derivation of eqn.30 relies on minimising the static potential elastic energy[37, 1], so it does not account for the kinetic energy. Lothe[392] and Stroh[27] examined this question, which was subsequently fully formalised by Mura[22]. They found that under dynamic conditions the Peach-Koehler force consists of two separate components.

The first matches eqn.30. The second is a *Lorentz term*, named in analogy with the Lorentz force of electrodynamics(Cf.[165]), and was examined in detail by Lund[393]. It takes the form[22]:

$$f_n^L = \rho \dot{u}_i \dot{\xi}_j B_i \epsilon_{jnh} \nu_h \tag{31}$$

where ν_h is the vector normal to the slip plane. This Lorentz term is perpendicular to the direction of motion, so (as its electrodynamic counterpart) it exerts no work[393]. Since the Lorentz force does no work it does not contribute to the energy transfer to the crystal lattice when the dislocation moves. Therefore it plays no role in the balance between the PK force and the drag force. The Lorentz term is a mathematical curiosity, and eqn.30 is the only relevant force under dynamic conditions.

5.2 Phenomenological mobility laws

Phenomenological laws are simple fits to data relating the applied remote shear stress τ and the steady state velocity of the dislocation. For low speeds, it is possible to produce phenomenological models from experimental data (see section 2); mobility laws for higher speeds typically rely on data extracted from atomistic simulations of the sort reviewed in section 4.2.

Gilman[394] argued that the best fit to experimental data on the velocity-stress relation was of the form:

$$v = v_0 e^{-\frac{d}{\tau}} \tag{32}$$

where d is a constant drag coefficient, and v_0 a limiting speed of the dislocation as the stress approaches infinity. In subsequent work, he[47] proposed a sigmoid function to better model the expected saturation at the speed of sound[47],

$$v = v_0(1 - e^{-\frac{d}{\tau}}) \tag{33}$$

When $v_0 = c_t$, eqn.33 saturates at the transverse speed of sound.

As an alternative that also saturates at the speed of sound, Gillis et al.[395, 396] proposed modifying the stress opposing dislocation motion so as to reproduce the relativistic behaviour predicted by Frank[10] and Eshelby[190]. The model, apparently originally due to J.W. Taylor (vid.[84]), modifies the drag coefficient to:

$$d = \frac{d_0}{1 - v^2/c_t^2} \tag{34}$$

where d_0 is the drag coefficient for dislocation motion at low speeds. Different versions of this approach have been introduced subsequently [395, 397, 398, 277, 399, 400, 401, 402], usually focusing on the exponent n of the term $(1 - v^2/c_t^2)^n$ in the denominator in eqn.34 to produce better fits. Common values include $n = 1/2$[395, 398, 277], $n = 1$[84, 354], and $n = 3/2$[403].

For the thermal activation and easy glide regimes[404, 405], power law relations have also been used:

$$v = v_0 \left(\frac{\tau}{\tau_0} \right)^m \tag{35}$$

Here, m is the slope of the $\log v - \log \tau$ curve (e.g., see fig.3), reported to be $m > 1$ for high speed dislocations[2]. Suggested low speed values of m for a number of materials can be found tabulated in [139]. These relationships are problematic for high speeds, both owing to the extraordinary non-linearities implied by $m \gg 1$, and because they fail to capture the existence of a limiting speed to the motion of dislocations (cf.[2]).

5.2.1 Inertial forces

Inertial forces explicitly compute the contribution to stress opposing dislocation motion (i.e., the '*drag*') due to the changes to the dislocation's self-energy as it accelerates. This 'drag' is usually referred to as 'radiative damping', and can be estimated using elastodynamics [217, 406, 257] as the energy radiated by a moving dislocation in the form of elastic waves.

Almost invariably, the calculations of radiative energy losses lead to an *inertial force* of the form

$$f_{\text{inertia}} = m\frac{\mathrm{d}v}{\mathrm{d}t} \tag{36}$$

where the factor m is generally called the (effective) *mass* of the dislocation [33, 407]. The dislocation's inertial force is not an inertial force in a Newtonian sense, since the mass of a dislocation must necessarily be dependent on velocity in order to account for the radiative energy losses (cf. [408]). Indeed, the 'mass' can be given the general mathematical form[409, 354]

$$m = \frac{1}{v}\frac{\partial H}{\partial v}, \tag{37}$$

where H is the self-energy of the dislocation. Most derivations of dislocation inertial forces focus on studying the form of m. The resulting f_{inertia} has the effect of opposing only changes to the dislocation's current speed.

5.2.2 The mass of a dislocation

As seen in eqn.37, calculating m requires finding the total self-energy H associated with an arbitrarily moving dislocation. The dislocation mass m was originally defined *ad hoc* in direct analogy with special relativity as [10]

$$m = \frac{m_0}{\sqrt{1 - v^2/c_t^2}} \tag{38}$$

where m_0 is the mass 'at rest', deduced as $m_0 = E_0/c_t^2$, where E_0 the elastic energy of a static dislocation (see [10, 1]). This term appears physically sensible: it should be about the mass of an atom divided by a bond length. For Al that is of order 10^{-16}kg/m. The self-energy of a dislocation is of order 10^{-9}J/m. Taking c_t to be 3000m/s we get $m_0 = 10^{-16}$ kg/m.

Following Weertman[168], Hirth, Zbib and Lothe [409] gave an alternative definition of the mass of a dislocation by using the self-similar elastic energy of the Frank-Eshelby moving dislocation. The lengthy expressions of this self-energy can be found in [229, 409, 354]. For an edge dislocations this energy is[354],

$$\begin{aligned} H^{\text{edge}} \quad = \quad & \frac{\mu b^2}{\pi M_t^4}\ln\left(\frac{R}{r_c}\right)\left[4\sqrt{1-M_l^2}\frac{M_t^2}{2} - 4\frac{1-M_t^2/2}{1-M_t^2} + \right. \\ & \left. + \frac{(1-M_t^2/2)^2}{2}\left(\sqrt{1-M_t^2} + \frac{6}{\sqrt{1-M_t^2}} + \frac{1}{\sqrt{1-M_t^2}^3}\right) + \frac{M_l^6}{2M_t^2\sqrt{1-M_l^2}}\right] \end{aligned} \tag{39}$$

where $M_l = v/c_l$, and R and r_c the dislocation's outer and inner core widths, respectively (see [1]).

As can be seen in eqn.40, Hirth, Zbib and Lothe's approach relies on the energy of a self-similar solution, which is an invariant of the motion (see section 3.2). The steady state dislocation neither radiates nor can change its kinematic state. Hence, employing a self-similar self-energy provides an unlikely model for dislocation inertia as it is generally understood. The ensuing Hirth-Zbib-Lothe (HZL) dislocation mass (obtained by applying eqn.37 to the self-similar expressions of H, q.v.[409]). For instance, for the edge dislocation it is given by:

$$m_{\text{edge}} = \frac{\mu B^2}{4\pi}\ln\left[\frac{R}{r_0}\right]\frac{c_t^2}{v^2}\left[-8\gamma_l - \frac{20}{\gamma_l} + \frac{4}{\gamma_l^3} + 7\gamma_t + \frac{25}{\gamma_t} - \frac{11}{\gamma_t^3} + \frac{3}{\gamma_t^5}\right] \tag{40}$$

where $\gamma_l = \sqrt{1-\frac{v^2}{c_l^2}}$, $\gamma_t = \sqrt{1-\frac{v^2}{c_t^2}}$. The HZL mass cannot be regarded as a true dislocation mass: at best, it provides an informed estimate of the difference in elastic energy levels between two dislocations moving at different speeds[354]. Compared to more sophisticated accounts, it also appears to considerably overestimate the dislocations' acceleration times[354].

Clifton and Markenscoff[35], building on work by Freund[410], showed that the energy radiated by a uniformly moving dislocation moving from rest at $t = 0$ was independent from the enclosing surface used to evaluate it.[8] This enables a simple estimate of both the energy and the associated mass of a dislocation. The energy radiated by the dislocation through an arbitrary surface S_d that encloses its core is

$$\dot{H} = \int_{S_d}\left[\sigma_{ij}n_j\dot{u}_i + \left(\frac{1}{2}\sigma_{ij}u_{i,j} + \frac{1}{2}\rho\dot{u}_i\dot{u}_j\right)v_n\right]\mathrm{d}S_n \tag{41}$$

[8] It must be noted that the same is not true for non-uniformly moving dislocations, which are subjected to a logarithmic singularity[217].

where σ_{ij}, u_i, $\dot{u}_i$ are the particle stress, particle displacement and particle velocity fields, v_n the dislocation velocity in the direction normal to the surface normal $\vec{n}$. Owing to the independence of S_d, it follows that

$$\dot{H}_0 = \lim_{S_d \to 0} \dot{H}, \tag{42}$$

which leads to the Markesncoff-Clifton (MC) inertial force:

$$f_{\text{inertia}} = -\frac{\dot{H}_0}{v} \tag{43}$$

The full expressions for $\dot{H}_0$ can be found in [217]. For an edge dislocation, it is given by

$$\dot{H}_0^{\text{edge}} = -\frac{\mu B^2}{2\pi}\frac{1}{t}\left[\frac{12 - 8M_l^2}{M_t^2\left(1 - M_l^2\right)^{1/2}} - \frac{(2 - M_t^2)(6 - 7M_t^2)}{M_t^2(1 - M_t^2)^{3/2}} - 2\left(1 - \frac{M_l^2}{M_t^2}\right)\right] \tag{44}$$

The inertia force then follows from eqn.43. We must note that irrespective of the dislocation's character, this $\dot{H}_0$ is proportional to $1/t$: it decays over time (see eqn.44). Crucially as well, eqn.44 (and its screw counterpart) become singular at the transverse and longitudinal speeds of sound, which in this model remain limiting speeds.

The expressions above rely on the path independence for S_d, which can only be achieved for uniform motions. The existence of an 'inertial' force when the motion is uniform is unlike the inertial behaviour expected in Newtonian mechanics. The inertial force in the case of uniformly moving dislocations exists because the dislocation began its motion from rest, so it necessarily radiates energy in the form of elastic waves, which arrived at retarded times on any material point. An arbitrary surface S_d enclosing the core would detect a decaying energy flux over time, as information about the dislocation's new velocity propagates through the material; the presence of a net energy loss manifests itself as an 'inertia' (eqn.43). To put it otherwise, it is because the material 'remembers' a time when the dislocation was not moving that an uniformly moving dislocation experiences an inertia-like force.

In non-uniform motions, the problem of estimating f_{inertia} becomes one of considerable complexity. A number of solutions have been proposed to produce a fuller account of inertia for that case. Markenscoff and Ni[264] were able to achieve an exact closed-form solution of the energy radiated by a non-uniformly moving screw dislocation with a ramp-like core (not reproduced here). This enabled them to reach a regularised expression of the dislocation mass for screw dislocations that was non-singular at the transverse speed of sound, thereby allowing for transonic motions. An analogous expression for edge dislocations is not yet available. Concurrently with prior work by Markenscoff[406], this work showed the crucial role the dislocation core plays in preventing trans- and supersonic motion, and how its regularisation (in this case via a fixed ramp) would affect the inertia term in the dislocation mobility law.

The issues surrounding the dislocation core, its width and its possible change with icnreasing speed had already been hitned at by Eshelby[411]. A more complex account of the inertial force, which allows for both changes in the core width with increasing dislocation speed as well as for radiative damping, was proposed by Pellegrini [256, 257] employing his own dynamic Peierls-Nabarro formulation[254], and building on previous work by Pillon et al. [258]. Of considerable mathematical complexity, Pellegrini's inertial force (see eqn.40 in [257]) accounts for self-energy losses and the variation in the core's width. It remains to to date the most physically insightful inertial force available. Furthermore, by regularising the core, it avoids singularities at the speeds of sound, allowing for supersonic motions[257]. Pellegrini's inertial model includes the radiative damping effect by construction, but the energy loss resulting from any other damping effects must be included phenomenologically, or rely on alternative models.

5.3 Inertial mobility laws and dynamic drag

The inertial force provides the dislocation with an acceleration pathway, which is unavailable under phenomenological drag forces. However, the acceleration time provided by inertial force estimates tends to be very brief. Using Frank's mass, Gilman[47] and Gillis and Kratochvil[396] estimated it to be of the order of 1ps, and inversely proportional to the magnitude of any additional dissipative mechanism present[47]. Gurrutxaga-Lerma[354], exploring the relative effect of the inertial forces described in section 5.2.2, also found that the inertial contribution vanishes in less than 10 ps as the dislocation approached it terminal velocity. The effect of the inertial term in determining the acceleration time is crucial: fully time-dependent expressions of inertia such as those provided by Pellegrini[257], Pillon et al.[258], or Markenscoff and Ni[264] tend to offer acceleration times that are about an order of magnitude smaller than those attained via steady state dislocation 'masses' such as the HZL mass.[354] It therefore seems that inertia on its own is an insufficient ingredient of dislocation mobility.

Furthermore, as noted by Gurrutxaga-Lerma[354], inertial forces vanish once the dislocation has accelerated, so their terminal speed can only be established by balancing the PK force with some alternative dissipative mechanism. For this reason, drag forces, usually proportional to the glide speed, appear as a constant companion to the inertial forces. These forces account for non-inertial dissipative mechanisms, usually in a semi-phenomenological way.

5.3.1 Sources of dynamic drag

The potential sources of non-inertial dislocation drag have been reviewed numerous times in the past by, amongst others, Gilman[47], Nabarro[140], Meyers[2], Granato[412], Hirth and Lothe[1], Ninomiya[413], Alshits and Indebom[50], Alshits[144], Nadgornyi [107] Galligan[414]. Table 1 summarises a (non-exhaustive) list of proposed drag mechanisms relevant at high speeds.

Source of drag	Physical mechanism	References
Inertial (radiative) effects	Drag caused by the emission of elastic waves by an accelerating dislocation.	[11, 169, 10, 107, 35]
Phonon viscosity	The moving dislocation's shear strain field displaces the phonon distribution. This is attenuated over time by the interactions between phonons, which can transfer energy between the transverse and longitudinal phonon modes, resulting in a net energy loss as the phonons relax to equilibrium	[415, 416, 417, 418, 419]
Electron viscosity	Analogous to phonon viscosity, but involving elastic scattering of electrons.	[420, 421, 422, 423]
Phonon scattering	The elastic field of the moving dislocation strains the atoms away from the perfect lattice positions.	[40, 424, 425, 426, 427, 428, 50, 429]
Electron scattering	The dislocation interacts with the electrons it encounters in its motion by inducing an electronic current that dissipates energy.	[109, 430, 407]
Thermoelastic damping	The hydrostatic fields of the moving dislocation may induce an irreversible thermoelastic heat flow between regions of tension and compression.	[431, 432, 107]
Solute drag	Drag due to the displacement of solute atoms dissolved in the lattice.	[190, 433, 434, 435]
Lattice friction	The potential energy of the dislocation changes in a periodic manner as it moves through the lattice, which results in an oscillatory force that dissipates energy.	[436, 437, 438, 439, 440, 114]
Other sources	Excitons, spin waves, grain and phase boundaries, quantum tunnelling,. . .	[84, 441, 442, 443, 444, 445, 446, 447]

Table 1: Different sources of drag acting on moving dislocations.

The relative importance of at least some of the mechanisms summarised in table 1 remains experimentally untested, and the range of speeds and applied strain rate levels over which they become relevant, or indeed, whether they are relevant at all, is a matter of ongoing research.

Some of them appear negligible even on theoretical grounds. For example, Weiner[432] concluded that thermoelastic dissipation did not seem to entail vast amounts of energy dissipation, and Gurrutxaga-Lerma[448] found that because the typical thermomechanical coupling constant in metals is small that volumetric changes entailed by fast moving dislocations did not translate in any sizeable temperature increase nor heat flow.

Other sources of drag have a corpus of well-attested experimental evidence, such as phonon scattering by dislocations (either elastic or inelastic), which can be measured in the acoustic attenuation displayed by the material (e.g., [112, 449, 450, 451]). Phonon scattering (elastic or inelastic) is believed to be the result of lattice anharmonicities[452] and the flutter mechanism[426, 437, 453, 454, 318, 455, 428, 456, 457] caused by the emission of elastic waves by the (thermal) vibrations of the dislocation line itself. The flutter mechanism predicts a drag contribution linearly proportional to the dislocation's speed[426, 437]. It appears to be important mainly at high temperatures, and most studies of the latter have focused on the temperature dependence of the ensuing drag coefficient (q.v.[437, 458, 116, 1, 459, 460]). On the other hand, the role of anharmonicities seems particularly testable at low temperatures. Anderson and coworkers [461, 462, 429] for instance provided direct experimental evidence that at low temperatures, dislocations in LiF are more effective at scattering slow phonons than fast ones. Moreover, as we discuss below, phonon scattering due to lattice anharmonicities is amenable to theoretical studies accounting the effect high speed dislocations. The effect of electron drag has also been estimated through indirect experimental evidence [463, 464, 135, 465].

The implications of some of the drag mechanisms can sometimes be observed in the macroscopic response. For instance, the electro- and magnetoplastic effects (q.v. [466]), whereby enhanced plastic flow is observed under strong electromagnetic fields[467, 135, 468, 469, 470] or in pure superconducting states[471, 464, 472, 473, 474, 475, 476] encountered at very low temperatures, have been associated with a relatively weak electronic drag and inertial effects governing dislocation motion[136, 137]. Indeed, Granato and coworkers[136, 137, 477] argued was brought about by inertial effects dominating dislocation motion because the dislocation would be underdamped in the absence of a sufficient phonon density at such low temperatures. Remarkably, they were able to show that the maximum in the dependence of the yield point with temperature found in superconducting states[478] could be explained via these inertial effects.

Equally, phonon scattering seems to have noticeable macroscopic effects under dynamic loading conditions. Indeed, it leads to a viscous-like drag force acting on the moving dislocation which may be expressed as[1] $f_{\text{drag}} = d \cdot v_{\text{dis}}$, where the drag coefficient d can be shown to be proportional to temperature, $d \propto T$[140, 114, 144]. This would suggest that a material deforming in a regime where dislocations are under free glide would experience thermal hardening. A considerably corpus of experiments carried out in the last two decades by Zaretsky and Kanel in a vast number of metals[479, 480, 481, 482, 483, 484] loaded at strain rates above 10^6s^{-1} show that many cubic and hexagonal metals do indeed display thermal hardening, giving further credence to a viscous drag-dominated dislocation mobility regime, and to its physical relevance[485].

In the following, we comment on a number of dislocation drag mechanisms that can be estimated for high speed dislocations.

Phonon and electron viscosities. Phonon and electron viscosity result in viscous drag-like coefficients that Mason estimated to be, respectively[415, 420, 416]

$$d_{\text{phonon}} = \frac{B^2}{8\pi r_0^2}\eta, \quad \text{and} \quad d_{\text{elect}} = \frac{(BN_e e)^2}{24\pi\sigma_e} \tag{45}$$

where r_0 is a nominal core cut-off radius, η the material's phonon viscosity, N_e the number of electrons per unit volume, e the electron charge, and σ_e the electrical conductivity.

Figure 15 reproduces the phonon and electron viscosities computed by Mason[421] for dislocations in Pb. The electron viscosity is small except for very low temperatures, where electrical resistivity is very low[412, 2], whereas phonon viscosity is relevant only at moderate and high temperatures.

Albeit qualitatively correct, Mason's theory overestimates dislocation drag by one or two orders of magnitude[140], particularly at low temperatures. Furthermore, this viscosity drag appears insufficient to account for high speed effects without further modification, which we do in the sequel.

Thus, let us take Frank's steady state solution for the displacement field of a screw dislocation:

$$u_z = \frac{B}{2\pi}\arctan\left[\frac{\gamma_t y}{x - vt}\right], \qquad \dot{u}_z = \frac{B}{2\pi}\frac{\gamma_t v y}{(x-vt)^2 + \gamma_t^2 y^2} \tag{46}$$

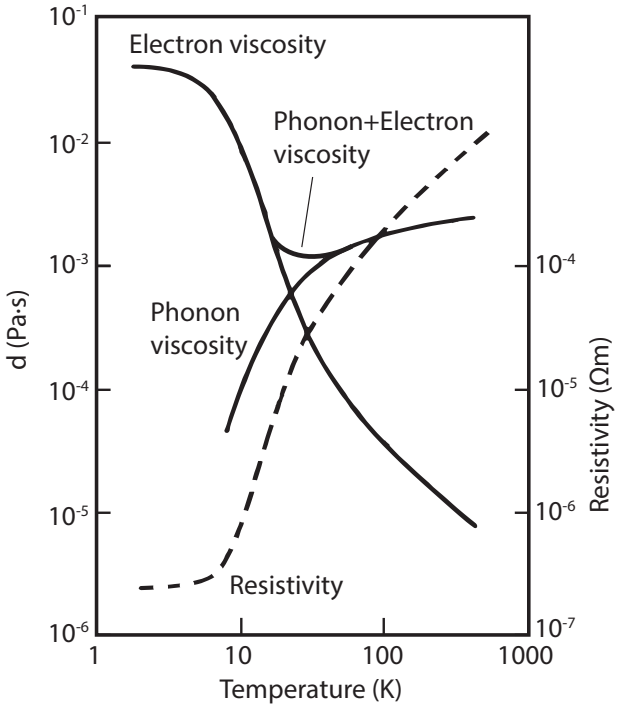


Figure 15: Predicted drag coefficient in Pb due to electron and phonon viscosity. Adapted from Mason[486].

Following Mason[415], for a medium with a viscosity η, the rate of energy dissipation is

$$\dot{q} = \frac{1}{2}\eta \left[\left(\frac{\partial \dot{u}_z}{\partial x} \right)^2 + \left(\frac{\partial \dot{u}_z}{\partial y} \right)^2 \right] \tag{47}$$

Integrating over all $\mathbb{R}^2$ for $x - vt$ and y, it is easy to show that the energy dissipated per unit length is

$$Q = \frac{B^2 v^2 (1+\gamma_t^2)\eta}{8\pi} \int_{r_0}^{\infty} \frac{\mathrm{d}r}{r^4} = \frac{B^2 v^2 (1+\gamma_t^2)\eta}{24\pi r_0^3} \tag{48}$$

where r_0 is a certain cut-off radius which Mason took to be about $r_0 = B/6$[415, 416]. Following Mason[415], if we equate $Q = \tau \cdot v$, we reach a drag coefficient of the form

$$d_{\text{relativistic}} = \frac{B^2}{24\pi r_0^3} \left(2 - M_t^2\right) \eta \tag{49}$$

where $M_t = v/c_t$ is the transverse Mach number.

The form of eqn.49 suggests that the phonon viscosity's contribution to the dislocation drag ought to decrease as the dislocation approaches the speed of sound: a fast enough dislocation would not give time for the viscosity-inducing phonons to relax back to equilibrium.

The effect of electronic drag, of considerable complexity, was reviewed by Alshits[144]. It is generally believed that electronic drag is of importance only at low temperatures. Its magnitude is believed to be directly proportional to the square root of the Fermi energy level E_F in the metal[487, 144], As is shown in fig.15, it is believed electronic drag is weak (of the order of 10^{-5}Pa·s), but that it increases with decreasing temperature[488, 489, 113], because it is thought to linearly dependent with the mean electron free path, that is expected to increase with decreasing temperature[144]. No expressions for high speed dislocations appear to be available, so we can only postulate that it follows a similar relationship to that derived in eqn.49.

Phonon scattering. Starting with Klemens[425] and Carruthers[490], several researchers including Alshits and collaborators[460, 459, 491, 427, 144], Li et al.[492], Blaschke[493, 145, 146] and Kim et al.[494] have worked on sophisticated analytical estimations the magnitude of the drag coefficient due to phonon scattering by dislocations.

These models usually rely on discrete and fully dispersive lattices, where the dislocation is modelled either as an explicit disregistry or as a moving discontinuity, and the net energy radiated by the core and scattered through its interaction with the lattice phonons are explicitly computed. Of considerable mathematical sophistication, all these theories seem to support the view that at least transonic motion is possible, and provide informed estimates of the drag coefficient. In particular, as shown by Blaschke et al.[146], at high speeds the drag coefficient can be estimated to take the form:

$$f_{\text{drag}} = d \cdot v, \qquad d_{\text{edge}} \propto \frac{1}{\sqrt{1 - M_t^2}}, \quad d_{\text{screw}} \propto \frac{1}{c_t} \tag{50}$$

Full expressions of the drag are given in [493, 146]. We note that the drag coefficient of edge dislocations increases in magnitude as the dislocation speed approaches c_t, but that of screw dislocations does not, which qualitative matches MD simulation data reviewed in section 4, whereby edge dislocations alone tend to display a saturation 'plateau' in the mobility below c_t. Nevertheless, in this account, the divergence of the drag term at the transverse speed of sound is seemingly brought about by the use of the steady state elastic field of the Frank-Eshelby dislocation in its derivation, which diverges at $v = c_t$ (see section 3.3), so it is unsurprising that the ensuing drag coefficient would display the same asymptotic behaviour as c_t is approached. Further analyses under anisotropic conditions have also been provided by Blaschke[145], highlighting the importance of the character of the dislocation segment, and the crystallographic orientation of the motion. In a less physically motivated model, Rosakis [495] proposed a semi-phenomenological drag force that accounts both for phonon scattering and *radiative damping*, which also showed energy divergences at the shear speed of sound.

The value of studying dislocation drag from a theoretical standpoint is in providing qualitative explanations of the different phonon-dislocation mechanisms active and relevant at high speeds: the increased role of radiative damping[494, 257] and phonon scattering effects[145, 144], for instance, as well as the importance of dislocation character and slip directions[145, 146], are crucial insights offered by these theories. Phenomenological models rely on constitutive assumptions that, as is the case with the hypothesis that a sound barrier for dislocations exists, remain contentious or contestable. Theoretical models need not rely on such assumptions, and can be used to provide better estimates of the mathematical form of the drag coefficient.

However, it is important to remark that both theoretical and experimental accounts of drag at high speeds remain largely unexplored, as most studies have focused on low speed phenomena (see [144, 1]) that are more easily compared to the existing body of experimental results (see section 2). It is hoped that the development of more sophisticated *in-situ* imaging techniques will finally enable direct observation of high speed dislocations that may facilitate the testing of the many theoretical assumptions embedded both in the modelling of the drag force and the inertial forces.

6 Conclusions and outlook

The interest in the study of high speed dislocations lies in their dominant role as the agents of plastic deformation under 'extreme' conditions; extreme here is used in the sense that the loading is considerably faster or more intense than in conventional "static" plastic flow, and where high speed dislocations may be present. A vast number of phenomena can be included in such category, such as plastic relaxation processes under shock loading[238, 496, 497, 387], dynamic fracture[498, 499, 500, 501, 354] and crack growth under dynamic conditions[502, 503, 504], shear band formation [505, 506, 507, 4], spallation [508, 509, 510, 511] and fragmentation[512, 513, 514, 515], dynamic contact[516, 517, 518], geophysical modelling of cracks and faults[519, 520, 521, 522]. These are all deformation and failure processes typical of e.g. defence and aerospace applications, crashworthiness of vehicles, seismology, and precision manufacturing processes.

Such applications would benefit from design rules and diagnosis techniques informed by a proper understanding of the mechanics and physics of high speed dislocation. However, it is fair to conclude that after almost 70 years of research into the phenomenology associated with fast moving dislocations, definitive conclusions remain elusive. This probably stems from a complete lack of experimental evidence regarding high speed dislocations, which makes their observation all the more necessary. It is to be hoped that in the near future, the new generation of synchroton light sources (e.g.[523, 524]) will provide sufficient spatial and temporal resolution to enable *in-situ* observations of fast moving dislocations. This will help settle the debate of whether dislocations can exceed the speed of sound, and pave the way for a new generation of measurements of dislocation mobility that supersedes those currently in use, the theoretical postulates of which, made in the 1960s and 1970s, are yet to be verified.

As argued in this review, the lack of experimental observation of high speed dislocations means that all that is known about them is supplied by theory and simulations. The dominating theoretical approach relies on the linear theory of elasticity, which *a priori* postulates that high speed dislocation motion saturates as the transverse speed of sound is approached, with this speed an insurmountable barrier. As has been discussed, this result is heavily reliant on the

symmetries embedded into the motion of a Volterra dislocation and of the governing equations of linear elastodynamics. Even within this continuum framework, it is possible to build models where there is no apparent sound barrier: a number of studies concerning the modelling of the dislocation core successfully show that the divergence at the speed of sound vanishes upon mollifying the dislocation core.

The historical motivation for most of these models was Gumbsch and Gao's [157] molecular dynamics simulations of transonic (and supersonic) dislocation motion. Although these simulations seemed to contradict linear elasticity, trans- and supersonic motion had already been shown to be possible in harmonic lattice models of moving dislocations. However, under the harmonic approximation a number of *breakdown velocities* appear, in which the dislocation core traps all energy it would otherwise radiate outwards. This leads to resonances and, potentially, to a *kinematic generation* mechanism[155, 159] triggered at very specific speeds: namely, when the dislocation glides at the bifurcation between the phase and group velocities of the dispersive lattice.

Although the harmonic lattice models provide a physical rationale as to why transonic and supersonic dislocations ought to be possible, the breakdown velocities typically occur below $\approx 0.3c_t$, which made them the subject of much criticism. This makes the results extracted from the far richer molecular dynamics simulations the preferred route to study high speed dislocations. In these simulations, the system may be thermalised, and anharmonicities can be included via physically richer interatomic potentials. As in harmonic lattice models, MD simulations may display breakdown velocities leading to kinematic generation[159]. Paradoxically, this suggests that these two features of high speed dislocations (supersonic dislocations and kinematic instabilities) are mediated by the discreteness of the atomic lattice, not by anharmonicities. However, the dispersion of energy away from the core, which manifests itself in the form of a drag force on the dislocation, will undoubtedly be governed by considerations beyond the mere discreteness of the lattice alone.

Thus, although molecular dynamics studies provide a semi-empirical way of studying high speed dislocation motion, to develop a general theory of high speed dislocation mobility has proven elusive. This is made all the more difficult by the nature of the drag dislocation motion is subjected to, which entails a vast number of possible mechanisms acting concurrently, from the elastic and inelastic scattering of phonons, to the radiation of elastic waves, ... In some cases, for example, with the lack of electronic effects and electronic conduction, these mechanisms may fall beyond the capabilities of molecular dynamics simulations. Equally so, MD models tend to be physically too rich, making it difficult to distinguish the different phenomena that contribute to the dislocation drag. Without a clear distinction, the resulting model of dislocation mobility would be entirely phenomenological, and devoid of the theoretical inputs necessary to facilitate their transferability and generality to materials of a similar class. Given that phonon drag and radiative damping are believed to dominate at high speeds, and that both phenomena are agreeable to study using discrete lattice dynamics models, it seems possible to provide general qualitative insights into the dislocation–lattice interaction, which has so far eluded the more physically rich MD simulations, that these models could complement.

Even then, molecular dynamics or similar atomistic studies may serve to provide a description of dislocation mobility, but not so much of how such high speed dislocations behave collectively. Thus a long-standing question regarding high speed dislocations remains: how do they interact with one another and with the medium, and how does their collective response — the high speed dislocation *plasticity* — differ? As argued in this review, in studying this part of the problem linear elasticity appears to be sufficient, for it serves to capture their long range interaction via the elastodynamic fields of the dislocations. The resulting model of plasticity is dominated by inertial effects, with retardations and Doppler-like magnifications in the interactions governing the plastic response. This constitutes a radically different paradigm of plasticity to the one that is usually found in quasi-static plasticity. Some phenomena dominating the response of metals subjected to high strain rates, such as the attenuation of the dynamic yield point[238] or the increase in the dynamic fracture toughness[240], seem to be the result of this dynamic picture of plasticity. However, a number of long-standing problems of static plasticity, namely the homogenisation of the collective response of dislocations and related statistical effects, still need to be explored under the assumption that dislocations structures are not in static equilibrium any more, and that interactions are based on a retardation principle. This constitutes an important shift in the approach to a problem that is *per se* paved with difficulties and largely remains unsolved. As a first step, it would be desirable for an elastodynamic analogue to the classical Orowan equation to be developed. This would at least provide a physical rationale for the development of adequate phenomenological constitutive laws that account for inertial effects.

This brings us to conclude that, in our opinion, there are three main issues that remain to be tackled and resolved by the many scientists and researchers who contribute to this field in the coming years. First, the development of techniques that enable direct empirical observation of high speed dislocations. Second, the realisation of a physics-based model of dislocation mobility that is transferable and general enough to be incorporated into design rules. Third, the establishment of a reliable model of high speed dislocation plasticity.

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