Misconceptions about Metals

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ABSTRACT: There are widespread misconceptions about the metallic bond and properties of metals in text-books and online resources in chemical education. This is surprising in view of the evident importance of metals and alloys in the modern World. Contrary to what is widely stated in the chemistry literature, Encyclopedia Britannica online, Wikipedia, ChatGPT, Google Bard and a recently published infographic on the Royal Society of Chemistry Web site, the electrostatic attraction between ion cores and free electrons in a simple metal is not sufficient to prevent it from disintegrating into its constituent atoms. It is also not true that localization of electrons is the reason for the difference between electronic conduction in metals and most insulators. The electrical resistance of metallic crystals is due to *deviations* from perfect structural and chemical order. The treatment in the same sources of processes within a crystalline metal when its shape is changed permanently bear no relation to experimental reality. Using almost no mathematics this article offers an insight at an accessible level into current thinking in chemistry and physics about metallic bonding and the properties of metals for teachers and students of chemistry in high schools and universities.

KEYWORDS: *Metals and Insulators, Metallic Bond, Covalent Bond, Electron Gas, Localized and Delocalized Electrons, Cohesion of Metals, Electrical Resistance, Malleability*

1. INTRODUCTION

Any course in chemistry would not be complete without a discussion of the nature and variety of chemical bonds. When students first encounter the chemical bond they learn it can be ionic, covalent or metallic, and simple descriptions of what these terms mean are discussed. Ionic and covalent bonding are relatively straightforward conceptually. Metallic bonding has been more problematic, and it has led to considerable confusion and misinformation in the literature and online resources. In this paper I have identified four pervasive misconceptions about the metallic bond and certain properties of elemental metals in the education of senior high school students and university undergraduates. For example, pages 160−161 of the text-book for the International Baccalaureate Diploma in Chemistry contain almost all the errors discussed below.^{[1](#page-5-0)} It is perhaps more concerning that the same errors exist on literally countless Internet sites, which may be freely accessed by teachers and students. They include the Wikipedia page on metallic bonding, the Encyclopedia Britannica online page on the metallic bond, the chemistrystudent.com Web site on the metallic bond, animations on YouTube, as well as ChatGPT and Google Bard. There is an infographic on the Royal Society of Chemistry Web site entitled "Everything you need to teach metallic bonding" where the same misinformation appears. It seems the misinformation has become folklore, despite the efforts of the late Jeremy K Burdett, who was Professor and Chairman of the Department of Chemistry at the University of Chicago, to correct much of it.^{[2](#page-5-0)} The aim of this paper is to explain carefully current understanding of the metallic bond and the most common properties of metals presented to high school students and undergraduates in chemistry. I hope teachers will be able to use this material directly in their classes, and that authors of curricula, text-books and online resources will make appropriate changes to their publications.

About three-quarters of the elements are metals. The Nobel Prize winning physicist Sir Nevill Mott defined a metal by its ability to conduct electricity at absolute zero.^{[3](#page-5-0)} The distinction between a metal and an insulator can be made only at absolute zero because the electrical conductivity of an insulator increases with temperature, although in common insulators the increase may be very small indeed.

The following misconceptions about metals may be found in elementary text-books and an uncountable number of online resources.

First Misconception:

In an insulator the outer shell electrons are *localized*, either on individual atoms forming ionic bonds as in sodium chloride, or between pairs of atoms in covalent bonds as in diamond. This localization of the outer shell electrons in an insulator renders them unable to conduct electricity. In contrast, the outer shell

Received: January 3, 2024 Revised: April 16, 2024 Accepted: May 29, 2024 Published: June 10, 2024

electrons of a metal are *delocalized*, so they are free to conduct electricity.

Second Misconception:

The ion cores of the metal are surrounded by the free electron gas. Since the ion cores are positively charged and the valence electrons are negatively charged they attract each other. Their attraction binds the metal together.

Third Misconception:

Resistance of metallic conductors is caused by collisions between electrons and positive ions of the crystal lattice.

Fourth Misconception:

The delocalized nature of bonding in metals enables planes of atoms to slide over each other relatively easily compared to insulators. Sketches in books and movies on the Internet show whole planes sliding *en masse* over each other. This is why metals are malleable and ductile whereas insulators are brittle. Metals are strengthened when impurities are added because the planes become distorted by the impurities and then it becomes more difficult for the planes to slide over each other.

In sections 2 to [5](#page-4-0) these misconceptions are discussed. In the concluding [section](#page-5-0) 7 four statements are proposed as corrections for the four misconceptions.

For the reader who wishes to explore the topics covered here in more depth there is a list of books in the [Supporting](https://pubs.acs.org/doi/suppl/10.1021/acs.jchemed.4c00010/suppl_file/ed4c00010_si_001.pdf) [Information](https://pubs.acs.org/doi/suppl/10.1021/acs.jchemed.4c00010/suppl_file/ed4c00010_si_001.pdf)

2. FIRST MISCONCEPTION

When chemists speak of localization of electrons in an insulator they mean they are confined either on an anion in an ionic material or in a bond in a covalent material. Another example is provided by core electrons, which are localized to a small region around the nucleus because they are unable to escape its strong attraction.

Chemists and physicists describe the valence electrons of a metal as being delocalized in the sense that they escape from the atoms, leaving behind positively charged ion cores, and moving freely throughout the entire metal, forming a "gas" of itinerant electrons.

Contrary to what is widely claimed in the chemical literature, only a small fraction of the itinerant electrons in a metal carry an electric current. To see why, consider a long thin metallic wire. Free electrons in the wire are in quantum states defined by their velocities to the left or right along the wire. The Pauli exclusion principle requires that each quantum state may hold no more than two electrons, one with spin up and the other with spin down. Each state is filled with an electron pair, starting from the lowest kinetic energy and ending with the highest kinetic energy $\frac{1}{2}mV^2$ until all free electrons in the wire have been allocated to states. Therefore, before an electric field is applied to the wire each quantum state in the range −*V* ≤*v* ≤ *V* is occupied by a pair of electrons, as shown in the lower row of states in Figure 1. As expected there is no net current of electrons in the wire before the wire is connected to a battery, because for every electron with velocity *v* there is another with velocity −*v*.

When the wire is connected to a battery *all* free electrons in the metal are accelerated toward the positive terminal. But they are accelerated for only a limited time *τ* before they are scattered by atomic vibrations, impurity atoms and structural defects such as missing atoms. The scattering is random, but we can treat it in an approximate way by assuming all the free electrons are accelerated for a time *τ* before their velocities are reset to zero

Figure 1. Schematic illustration of the change in the occupation of quantum states, labeled by the velocity *v*, when an electron current flows to the right in a long thin metal wire. Blue rectangles represent quantum states. Orange shading signifies states occupied by two electrons, one spin up one spin down. White rectangles signify unoccupied states. The lower row of states shows the equal occupation of states with ±*v* when there is no current flowing. The upper row shows the occupations of states when there is a current flowing to the right. The entire upper row of states is shifted to the right by Δ*V*. Electrons in states shaded green are the only ones carrying the current.

and the process begins again, as sketched in Figure 2. As we will discuss in [section](#page-3-0) 4 these scattering events are the source of electrical resistance of the metal.

Figure 2. Drift velocity of a current-carrying electron in a metal as a function of time. The electron is accelerated by the electric field between scattering events, which occur on average every *τ* seconds.

Let ΔV be the average change in the velocities of the free electrons between scattering events. The range of electron velocities between successive scattering events is then $-V + \Delta V$ $\leq v \leq V + \Delta V$. As illustrated in the upper row in Figure 1 the states between $-V - \Delta V$ and $-V$ are emptied and so do not contribute to the current. Electrons in the states between *V* − ΔV and $V + \Delta V$ carry all the current because there are no electrons in states with the opposite velocities between −*V* + Δ*V* and $-V - \Delta V$. The current-carrying states are colored green in Figure 1. The restriction that no more than two electrons can occupy a state prohibits changes to the occupations of the remaining states, and since they occur in pairs of states with ±*v* they carry no current. Consequently the current flowing in the wire is carried only by a small fraction Δ*V*/*V* of the free electrons in the wire. In practice $\Delta V/V$ is very much less than 1. We see that the Pauli exclusion principle has a dramatic influence on the electrical conductivity of metals.

The notion that insulators are not electronic conductors because their valence electrons are localized is misleading at best. Diamond is an excellent insulator. Each bond in diamond is saturated and contains two electrons. If the same two electrons were localized in a bond they would be completely decoupled from other bonds. Each bond could then be treated in the same way as the bond in a diatomic molecule, with a bonding state containing the two electrons and an empty antibonding state. Since all bonds in diamond are identical the valence electrons in diamond would have only these two energy levels, and they would all occupy the bonding state while the higher energy antibonding state would remain empty. But that is not what happens in diamond.

The reason why the covalent bonds in diamond are so strong is that the valence electrons are able to move easily not only between a pair of atoms forming a particular bond, but from an atom to any of its four neighbors, and hence throughout the entire crystal. In diamond valence electrons are just as free as the free electrons in any metal. The resulting itinerant nature of the valence electrons creates two bands of states in which their energies are in ranges centered on the bonding and antibonding states of the "diatomic molecule" of the previous paragraph. These energy ranges are called bands, and the lower energy band is called the valence band and the higher energy band is called the conduction band. In diamond the valence band is full because every state is occupied by two electrons. It is separated in energy from the conduction band by about 5.5 eV (530 kJ/ mol), which is called the band gap. The existence of these bands and the band gap has been confirmed experimentally using spectroscopic techniques.

If the valence electrons in diamond are just as free as those in any free electron metal why is not diamond a good conductor of electricity? It is because every state in the valence band is full. Unlike the change of state occupation in a metal depicted schematically in [Figure](#page-1-0) 1, when an electric field is applied to diamond there are no unoccupied states in the valence band available to accept an accelerated electron, because all the valence band states are fully occupied and prohibited by the exclusion principle from taking more than two electrons each. The only way an electron in pure diamond can conduct electricity is to cross the band gap and occupy one of the empty states in the conduction band. At room temperature the thermal energy available for such a transition is about 0.025 eV (2.4 kJ/ mol). The probability of such a transition is virtually zero. Diamond is an excellent insulator!

Electrons in most insulators are unable to carry a current because there is a finite energy, the band gap, separating occupied and unoccupied electronic states. But there are some materials where electron localization of free electrons does occur and it does lead to insulating behavior. The following is a thought experiment that cannot be realized in practice, but it does illustrate the point. Imagine what would happen if we could gradually increase the separation of sodium atoms arranged on its crystal lattice, starting from the equilibrium density of sodium metal and finishing with nearest neighbor sodium atoms one meter apart. We start with a metal and finish with an insulator. In the metal the 3s electron on each sodium atom is delocalized in the electron gas. But at some point, long before the nearest neighbor separation reaches one meter, the 3s electrons localize themselves onto the $Na⁺$ ion cores forming neutral sodium atoms. The metal then becomes an insulator because for an electron to be transferred from one neutral atom to another the first atom has to be ionized to Na^+ and the second to Na^- , which requires approximately 4.4 eV (425 kJ/mol) of energy.

3. SECOND MISCONCEPTION

There are two common classes of metallic bonding:

- (i) the "simple metals" dominated by sp-bonding, and
- (ii) the transition metals dominated by dd-bonding.

[Note: Bonding in the f-block metals (i.e., the lanthanides and actinides) has similarities to bonding in the transition metals. The main difference is that electrons in f-states have an even smaller spatial extent than those in d-states. This leads to stronger electron repulsion between electrons in f-states, which plays a central role in the chemistry and physics of f-block metals. Bonding in f-block metals is an area of current research.]

3.1. Simple Metals

In free atoms of simple metals the valence electrons are in s and p states only. The elements of groups 1, 2, and 13 and tin and lead in group 14 are examples of simple metals. Nearly all their cohesion is provided by a purely density-dependent, structureindependent energy. Differences in the energies of alternative crystal structures with the same density are much smaller, typically of order 1−10 kJ/mol. As a first approximation, bonding in these metals may be described by a model in which positive metal ions are immersed in a gas of delocalized valence electrons.

A moment's thought reveals that the second misconception is a very one-sided account of the energy balance associated with the creation of a simple metal from its atoms. The liberation of the valence electrons into the electron gas amounts to ionizing the atoms, which requires a great deal of energy. For example, in aluminum each atom contributes three valence electrons to the electron gas leaving behind an Al^{3+} ion. The first three ionization energies of aluminum amount to 5140 kJ/mol (53 eV per atom). That is more than ten times the cohesive energy of aluminum. In addition, the liberated electrons enter an electron gas where they repel each other electrostatically. They are also forced to have significant kinetic energy, even at absolute zero, to satisfy the Pauli exclusion principle. For the metal to be stable against separating into its constituent atoms these very large positive energies have to be offset by an even larger negative energy.

The attractive interaction between the ion cores and the electron gas is considerably weaker than might be expected from electrostatics alone. One reason for this is again the Pauli exclusion principle. An electron of the electron gas may penetrate an ion core. Since all the core states are already full the valence electron is forbidden from entering any of them. This forces the valence electron into a state of higher energy, which is equivalent to a repulsive interaction that weakens the Coulomb attraction to the nucleus. In fact the weakening of the attraction to the nucleus is so great inside the ion core it is virtually canceled. That leaves only the electrostatic attraction to the nucleus outside the core, but that is reduced by the electrostatic repulsion from the core electrons. So where does the required additional attraction come from that makes the metal stable?

The answer is that the valence electrons reduce their electrostatic repulsion by keeping out of each other's way. Sharing the same negative charge, the valence electrons repel each other electrostatically. That ensures they do not approach each other too closely. In addition to their electrostatic repulsion, electrons with the same spin also repel each other owing to the exclusion principle. The net result is that an electron in the electron gas of a metal is surrounded by a small exclusion zone into which other electrons rarely ever enter. The existence of the exclusion zones leads to a reduction in the overall electrostatic repulsion between electrons in the electron gas because they are prevented from getting too close to each other. These exclusion zones make an *essential* contribution to the stability of a metal.

3.2. Transition Metals

In the transition metal series the filling of the d-shell dominates cohesion, and it determines the systematic changes in crystal structure as we move across the 4d and 5d series. The same is true of the 3d series but the occurrence of magnetism is a complication. The differences in energy between competing Table 1. 3d, 4d and 5d Transition Metal Series Showing, for Each Element, the Crystal Structure, the Cohesive Energy *Ec* in kJ/ mol, the Melting Point *Tmp* in **°**^C and the Bulk Modulus *^B* in GPa*^a*

a
 a HCP = hexagonal close packed, FCC = face centered cubic and BCC = body centered cubic. 1 GPa = 10⁹ Pa, and 1 Pa is 1 Pascal, which is 1 Newton per square meter. Values in parentheses are estimates. Data from Kittel.^{[4](#page-5-0)}

crystal structures of a transition metal are again much less than its cohesive energy.

The transition metals are not described well by the free electron model of the previous section. The d-electrons in the outer shells of transition metals are more tightly bound to the nucleus than the outermost s-electrons. This reduces the overlap between d-orbitals on neighboring atoms, compared with outer shell s-orbitals. Nevertheless, valence electrons in transition metals are also delocalized throughout the metal. The valence dstates in transition metals form directional, unsaturated covalent bonds with their neighbors producing some of the largest cohesive energies of all the elements.

Table 1 shows the crystal structures, cohesive energies, melting points and bulk moduli of the 3d, 4d and 5d transition metals series. The bulk modulus determines the resistance of the metal to compression. The BCC, FCC and HCP crystal structures are shown in Figure 3. As we cross the 4d and 5d series

Figure 3. Common crystal structures of metals: body centered cubic (BCC), face centered cubic (FCC) and hexagonal close packed (HCP).

we see the cohesive energy, melting point and bulk modulus rise to a maximum in the middle of the series and then fall. These trends are less apparent in the 3d series owing to the occurrence of magnetism in Fe, Co and Ni.

The explanation for these trends is as follows. As we cross the series the d-states are being filled by electrons, from 1 on the left to 10 on the right. As the number of electrons increases from 1 to 5 they go into bonding d-states. In the middle of the series all the bonding d-states are filled and the antibonding states are empty. The bond strengths are then a maximum. Further filling of the dstates results in the occupation of antibonding d-states, which reduces the bond strengths. Consequently in the second half of the transition metal series the cohesive energy, bulk modulus and melting point all decrease as d-states are filled further. The decline in these properties in the second half of the series shows clearly they do not always increase with increasing number of valence electrons per atom, contrary to another pervasive misconception.

Notice the remarkable consistency between the changes of crystal structure as we cross the 4d and 5d series: $HCP \rightarrow BCC$ \rightarrow HCP \rightarrow FCC. This is a much more subtle trend because the differences between the energies of these crystal structures are much smaller than their cohesive energies. Nevertheless, it turns out it is directly related to the filling of the d-states.^{[5](#page-5-0)}

4. THIRD MISCONCEPTION

When an electric current flows in a metal the metal heats up. This happens because current-carrying electrons transfer some of their energy to ions in the crystal. These energy transfers occur at the scattering events mentioned in [section](#page-1-0) 2. It is a characteristic property of metals that their electrical resistance increases with temperature, because there is more electron scattering by thermal vibrations. In contrast, the resistance of an insulator decreases with increasing temperature because more electrons are excited thermally across the energy gap between occupied and unoccupied states.

The third misconception is misleading because it omits the essential point that electrical resistance of metals is due entirely to deviations from the periodic structure of the perfect crystal. A "perfect" crystal has no structural defects or impurities and its atoms are frozen in position to maintain *exact* periodicity. Through this omission the misconception implies that if the crystal were perfect there would still be resistance. However, there is a rigorous proof, called Bloch's theorem, that valence electrons travel completely unimpeded in a perfect crystal of a metal. In reality atoms in a crystal are never static, even at absolute zero, because that would violate the uncertainty principle. Therefore, a "perfect" crystal in the sense defined here cannot exist. Provided the metal does not become a superconductor, quantum physics shows the resistance remains finite

Figure 4. A dislocation loop lying in a slip plane separating slipped and unslipped regions. The dislocation is the line separating the slipped and unslipped regions of the slip plane. It forms a loop. Inside the loop the material beneath the slip plane has been displaced with respect to material above it by the vector **b**, which is known as the Burgers vector. From Sutton.^{[6](#page-5-0)}

even at absolute zero due to spontaneous emission of quantized atomic vibrations called phonons. Nevertheless, electrical resistance in a metal is *always* due to deviations from the idealized structure of a perfect crystal.

5. FOURTH MISCONCEPTION

Plastic deformation occurs when an applied load changes the shape of a material permanently. It differs from elastic deformation which is fully reversible when the load is removed. The ability to permanently shape metals is used throughout technology, including construction, transport, energy production and transmission, defense, communication, and much more. Plastic deformation does take place by atomic planes sliding over each other. The process of sliding is called slip and the planes on which it occurs are called slip planes. However, slip does *not* occur by entire planes of atoms sliding *en masse* over each other, as portrayed in the books, articles and online videos where the fourth misconception appears. Instead slip begins in small patches of a plane and the patches subsequently expand (see Figure 4). The boundary of a patch is a linear defect called a *dislocation*. *Plastic deformation in all crystalline materials involves the formation and movement of dislocations*. [Note: Some crystals deform plastically through the nucleation and growth of threedimensional sheared regions called "deformation twins". However, even these defects involve the creation and movement of dislocations.] There are movies on the Internet of dislocations moving in crystals, as seen in a transmission electron microscope, e.g. see [https://www.youtube.com/watch?v=](https://www.youtube.com/watch?reload=9&v=BV1cxwxnhPs&ab_channel=OndrejKotecky) [BV1cxwxnhPs&ab_channel=OndrejKotecky.](https://www.youtube.com/watch?reload=9&v=BV1cxwxnhPs&ab_channel=OndrejKotecky) An excellent model of dislocations and other defects in crystals is the bubble raft, although it is only two-dimensional, e.g. see Sir Lawrence Bragg's beautiful video of a bubble raft at [https://www.youtube.](https://www.youtube.com/watch?v=UEB39-jlmdw) [com/watch?v=UEB39-jlmdw.](https://www.youtube.com/watch?v=UEB39-jlmdw) For an elementary introduction to dislocations see Hull and Bacon.^{[7](#page-5-0)}

The strength and degree of directional bonding does affect the mobility of dislocations and hence the malleability of the material. But there are other factors, at least as important, such as the ambient temperature, alloying, and the history of thermal

and mechanical treatments to which the material has been subjected. It is the interaction between dislocations and impurity atoms that determines how impurities affect ductility.

Some metals are malleable at room temperature but brittle at low temperatures. As the temperature is raised they pass through a 'brittle to ductile transition', whereupon they become ductile, but bonding between atoms barely changes. This experimental fact is a clear indication that the ductility of these metals and alloys is only indirectly related to bonding in them.

It is quite wrong to suggest that all metals are malleable. Some intermetallic compounds, such as $Al₃Ti$, FeAl, TiAl and MoSi₂, are brittle at room temperature. Iridium is an elemental metal with the same crystal structure as aluminum that becomes ductile only at temperatures above 700 °C.

It is also quite wrong to imply that all insulators are brittle. Some insulating crystals also display a brittle to ductile transition. For example, at room temperature silicon and diamond are brittle, but they display some ductility when the temperature is raised sufficiently.

In steels minute concentrations (parts per million) of antimony, tin, sulfur and phosphorus can lead to severe embrittlement without affecting bonding throughout the overwhelming majority of the material. Minute quantities of hydrogen embrittle many metals and alloys.

The relationship between the mechanical properties of materials and their chemical bonding is far more nuanced than the fourth misconception suggests. The mechanisms described in the misconception as being responsible for the malleability of metals and how they are strengthened by impurities bear no relation to experimental observations in any crystalline material.

6. DISCUSSION

Linus Pauling recognized in his influential book, *The nature of the chemical bond*, that the metallic bond is a type of covalent bond because they are both characterized by the sharing of electrons.^{[8](#page-5-0)} Covalent bonds, like those in alkanes and diamond, are *saturated* because they contain two electrons. They are strong and directional. Metallic bonds are *unsaturated* because

they contain less than two electrons. Bonds in transition metals are also strong and directional. Bonds in simple metals are weaker and less directional.

What does it mean to say a metallic bond involves sharing say 0.25 electron? This can be understood only as a time average value of the number of electrons shared in the bond. In Pauling's terminology valence electrons of a metal "resonate" between all bonds in the metal, such that over time the average number of electrons in the bond is 0.25.

If the number of nearest neighbors of an atom in a metal is *z* then the binding energy per atom may be written approximately as $E_B = Az - B\sqrt{z}$, where *A* and *B* are constants that depend on the nearest neighbor separation. The term *Az* represents a positive repulsive contribution and $-B\sqrt{z}$ is a negative attractive contribution. The square root dependence of the attractive contribution is a consequence of the unsaturated nature of metallic bonding. At a free surface the number of nearest neighbors is reduced. The attractive energy *per bond*, i.e. $B\sqrt{z}/z = -B/\sqrt{z}$, is larger in magnitude at a surface because there are fewer neighbors for valence electrons to resonate between. This is why bonds at a metal surface are generally stronger than in the bulk.

We have seen that the Pauli exclusion principle plays a central role in the properties of metals and insulators. Although its origins are in advanced quantum mechanics, students are usually introduced to it at an early stage in their learning when they encounter the structure of the Periodic Table and Hund's rules. It should be included in all teaching about electronic properties of metals and insulators.

7. CONCLUSIONS

Correction of First Misconception

Metals are defined by their ability to conduct electricity at absolute zero. Metals conduct electricity because there is no energy gap between occupied and unoccupied electron states. Most insulators do not conduct electricity at absolute zero because there is a finite energy gap between occupied and unoccupied electron states.

Correction of Second Misconception

The metallic bond is an unsaturated covalent bond formed by sharing less than two electrons in itinerant electron states. In simple metals, the attraction between ion cores and the electron gas is the dominant contribution to cohesion but it is insufficient to bind the metal together. Electron−electron interactions make an essential contribution to the cohesion of metals by reducing the electrostatic repulsion between electrons in the electron gas. In transition metals the dominant contribution to cohesion is the formation of directional unsaturated bonds involving electrons in d-states, the strength of which rises and falls with the filling of the d-band.

Correction of Third Misconception

Electrical resistance in metallic conductors arises when currentcarrying electrons transfer energy and momentum during scattering processes caused by deviations from the periodicity of the perfect crystal lattice such as atomic vibrations, impurities and structural defects.

Correction of Fourth Misconception

Many metals and alloys are ductile at ambient temperatures. However, some metals and alloys become brittle as the temperature is reduced, and some become brittle when they contain minute amounts of certain impurities. Some insulators

are brittle at low temperatures and become ductile when the temperature is raised. Ductility in all crystalline materials is determined by the mobility of dislocations, which can be engineered by alloying, heat treatments and interactions with impurity atoms.

■ **ASSOCIATED CONTENT**

s Supporting Information

The Supporting Information is available at [https://pubs.ac](https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00010?goto=supporting-info)[s.org/doi/10.1021/acs.jchemed.4c00010.](https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00010?goto=supporting-info)

Further reading ([PDF\)](https://pubs.acs.org/doi/suppl/10.1021/acs.jchemed.4c00010/suppl_file/ed4c00010_si_001.pdf)

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Notes

The author declares no competing financial interest.

■ **ACKNOWLEDGMENTS**

I am grateful to Tchavdar Todorov for helpful discussions, to Mike Finnis, Stan Lynch and Tony Paxton for their comments, and to a reviewer for stimulating comments and suggestions. I thank a high school teacher of the International Baccalaureate Diploma in Chemistry who first made me aware of the misconceptions discussed in this article.

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