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Atomic level computer modelling of crystal defects with emphasis on dislocations: Past, present and future

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ABSTRACT

Computer modelling is at present as important method of the study of materials and their properties as experiments. Yet, experiments have been being performed for several thousands years while computer modelling started about fifty years ago. In this introductory paper we first present a historical account of the advancement of computer modelling. Since defects in crystalline materials control most of their properties but their atomic level structure and properties cannot be treated analytically, they provided the impetus for the advancement of computer modelling in materials science. In between the plethora of defects we concentrate here on dislocations since it was established via modelling that it is the non-planarity of the cores of screw dislocations in BCC metals which controls their plastic properties. This understanding then lead to the recognition that the non-planarity of dislocation cores is common in many materials and frequently determines their properties. This atomic level aspect of dislocations is considered in more details, not only for the BCC metals, and relation to the macroscopic plastic behaviour discussed. Computer modelling plays, of course, important role in studies of many other defects, such as interfaces, surfaces, irradiation induced defects etc., as well as glasses and liquids, and the last part of the paper is devoted to discussing the possible future developments, in particular from the point of view of available descriptions of atomic interactions that are the precursor of any atomistic modelling.

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1. Introduction

It is fitting to start this brief account of atomistic modelling by quoting Professor Sir Charles Frank: *Materials are like people, they are interesting by their defects*. Indeed, majority of the properties of crystalline materials, in particular their mechanical behaviour, are controlled by defects such as dislocations, vacancies, interstitials, interfaces, surfaces and generally by regions that deviate away from the ideal crystal structure. In fact, the concept of defects has been introduced even for glasses in order to analyse their deformation and the glass transition [1,2]. Since the atomic structure and properties of crystal defects cannot be in general treated analytically, numerical computer modelling became an obvious tool for such studies as soon as computational physics appeared and at present it is as important part of materials science as the experimental studies.

The oldest atomistic computer simulations of defects in materials are, we believe, modelling of grain boundaries and related investigation of the dependence of their energy on grain misorientation [3], and study of irradiation induced cascades [4]. In the case of dislocations it is the study of dissociation of dislocations in FCC metals [5,6]. It became immediately obvious already in these early studies that the results depend strongly on the description of interactions between the atoms and, therefore, the development of appropriate representations of these interactions has been an essential ingredient in the advancement of atomistic modelling [7]. These descriptions range from empirical pair potentials, such as frequently employed Johnson's potential for iron [8], through many-body central-force potentials (EAM [9] and Finnis–Sinclair potentials [10,11]), quantum mechanics based approximate methods, such as bond-order potentials [12] (for several reviews see [13]) and/or potentials based on generalised pseudopotential theory [14], up to the calculations employing methods based on the density functional theory [15]. We shall not discuss in this brief outline any details of representations of interactions between the atoms and only mention their different contributions in the context of atomistic modelling.

Owing to their long range stress and strain fields, dislocations and their impact on plastic deformation of crystals have been analysed in great detail in the framework of the continuum elasticity. On the other hand, their atomic level properties, i.e. the core structure of dislocations, were for long time considered more as a scientific curiosity than a central property significantly impacting plastic behaviour of materials. This attitude changed when it was definitely established that $\frac{1}{2}[111]$ screw dislocations control plastic properties of BCC metals because of the non-planar character of their cores [16,17]. At present, it is fully recognised that the non-planarity of dislocation cores is very common in materials with not close-packed structures and that dislocation core effects play frequently a crucial role in deformation behaviour. This has recently been reviewed in [18] and several cases discovered by computer modelling are noted below.

2. Dislocation cores and stacking faults

2.1. Stacking fault-type defects

A vital characteristic of dislocations in crystalline materials is their possible dissociation into partial dislocations with Burgers vectors smaller than the lattice vector. Such dislocation splitting can occur if the displacements corresponding to the Burgers vectors of the partials lead to the formation of

metastable planar faults, which then connect the partials. This is well known to take place on $\{1\ 1\ 1\}$ planes in FCC materials and on basal planes in hexagonal materials. The lattice dislocations dissociate on these planes into Shockley partials and this is the principal reason why they are planar, confined to the plane of splitting, and for this reason the lattice resistance to their motion, the Peierls stress, is very low and does not affect significantly the yield or flow stress. In the early days of the studies of dislocations in BCC metals several possible stacking faults on $\{1\ 0\ 1\}$ and $\{1\ 1\ 2\}$ planes were proposed using the hard spheres model and dislocation dissociation with these faults considered albeit not necessarily as a planar splitting in the case of screw dislocations [19–22]. However, the major question always was whether metastable stacking faults exist in these metals since such faults have never been observed and the hard sphere model does not represent a stable BCC structure. This question was first tackled from the atomistic point of view by introducing the concept of γ -surfaces that are theoretical constructs on the basis of which metastable planar faults can be identified [23].

In order to introduce the idea of a γ -surface, we first define a generalised stacking-fault. Consider that the crystal is cut along a given crystallographic plane and the upper part displaced with respect to the lower part by a vector \vec{u} , parallel to the plane of the cut. The fault created in this way is called the *generalised stacking-fault* and it is not in general metastable. The energy of such fault, $\gamma(\vec{u})$, can be evaluated by atomistic modelling for a chosen description of interactions between the atoms; relaxation perpendicular to the fault has to be carried in such calculations. Repeating this procedure for various vectors \vec{u} within the repeat cell of the given crystal plane, an energy-displacement surface is constructed, and this surface is called the γ -surface. The positions of local minima on this surface determine the displacement vectors of all possible metastable stacking-fault-like defects, and the values of the energy at these minima are the energies of these faults. Symmetry arguments can be utilised to assess the general shape of these surfaces. If a mirror plane of the perfect lattice perpendicular to the plane of the generalised stacking fault passes through the point corresponding to a displacement \vec{u} , the first derivative of the γ -surface along the normal to this mirror plane vanishes owing to the mirror symmetry. This implies that the γ -surface will possess extrema for those displacements for which there are at least two non-parallel mirror planes of the perfect lattice perpendicular to the fault. Whether these extrema correspond to minima, and thus to metastable faults, can often be ascertained by considering the change in the nearest neighbour configuration produced by the corresponding displacement. Hence, the symmetry-dictated metastable stacking-fault like defects can be found out at a given crystal plane by analysing its symmetry. Such faults are then common to all materials with a given crystal structure regardless of the details of interactions between the atoms. The intrinsic stacking faults on $\{1\ 1\ 1\}$ planes in FCC crystals and on the basal planes in HCP crystals are such symmetry dictated faults since three mirror planes pass through the points that correspond to the fault displacements. However, other minima than those associated with symmetry-dictated extrema may exist in any particular material. These cannot be anticipated on crystallographic grounds, and their existence depends on the details of atomic interactions and can only be revealed by calculating the corresponding γ -surfaces.

Calculations of γ -surfaces for $\{1\ 0\ 1\}$ and $\{1\ 1\ 2\}$ planes, which were first done using empirical pair potentials and potentials derived on the basis of weak pseudopotentials for alkali metals [23], found no metastable faults. These calculations were repeated many times by a number of different authors using various descriptions of atomic interaction and the results were always basically the same: there are no single layer metastable stacking faults in BCC metals. An example of such recent calculation that employed a DFT based method is in Ref. [24]. This finding changed fundamentally the thinking about the core structure of screw dislocations in BCC metals that could not be analysed in terms of standard dislocation splitting but rather only by direct atomistic simulations.

2.2. Structure of the core of $\frac{1}{2}[1\ 1\ 1]$ screw dislocations in BCC metals

The first atomistic calculations of the $\frac{1}{2}[1\ 1\ 1]$ screw dislocation were carried out in [25,26]. Both these calculations employed pair potentials; empirical ones in the former and pseudopotential based potentials for alkali metals in the latter. In both these studies, and all the calculations that were done in the following 40 years, the core structure was found to be non-planar, spread principally into the three $\{1\ 0\ 1\}$ planes of the $[1\ 1\ 1]$ zone. It always retains the symmetry consistent with the threefold

screw axis of the $[1\ 1\ 1]$ direction, which is the consequence of the inability of the $1/2[1\ 1\ 1]$ screw dislocation to split into partials confined to one plane. However, in these studies and many following calculations employing central-force potentials, the core structure was found not to be invariant with respect to another symmetry operation, the $[1\ 0\ \bar{1}]$ diad. This implies that two degenerate structures, related by this symmetry operation, exist. In the projection onto the $(1\ 1\ 1)$ plane they appear as threefold but calling them threefold is not crystallographically correct. Nevertheless, this finding does not exclude that for some other descriptions of atomic interactions non-degenerate core structures, invariant with respect to the $[1\ 0\ \bar{1}]$ diad, exist. Indeed, such structures were found in all calculations for transition metals in which the directionality of bonding arising from the partially filled d-band has been taken into account [27–30] but also in some calculations employing central-force potentials [31,32]. The non-degenerate core has often been referred to as sixfold, which again is not crystallographically correct.

Nonetheless, the reason for investigation of the core structure is understanding of its effect on the plastic behaviour of single crystals and eventually polycrystals. Thus the next question is how the dislocations with the non-planar core structures move under the effect of applied stresses. This was first studied in [26,33] using pair potentials and since then in a broad variety of calculations (for a review see [18]). In most of these calculations, which were carried out at 0 K, the dislocation moves along a $\{1\ 0\ 1\}$ plane at stress of the order of 10^{-2} to 10^{-1} of the shear modulus. Hence, the Peierls stress is very high and, in fact, the calculated values exceed the experimentally measured critical resolved shear stresses extrapolated to 0 K by a factor of two to three. This problem has not yet been fully resolved although explanations taking into account the fact that many interacting dislocations always participate in the plastic flow have been suggested [34,35] and even the possibility of tunnelling of dislocations at low temperatures considered [36]. In all calculations the so-called twinning–antitwinning asymmetry of shearing was observed, which is in agreement with many observations, and was generally considered to be the source of all observed asymmetries of the yield and flow in BCC metals [17]. However, more recently it was found that the asymmetry arising from the effect of shear stresses perpendicular to the Burgers vector may be very large and in some cases superseding the twinning–antitwinning asymmetry [30–32].

The question that has been discussed up to the present time is whether the response of the degenerate and non-degenerate cores to an applied stress is very different and thus whether this difference in the cores may play a distinct role in different materials. As analysed in more detail in [37], under the effect of the applied stress the symmetry related to the $[1\ 0\ \bar{1}]$ diad is always eliminated and both cores attain a configuration akin to the degenerate structure with displacements spread most extensively into the $(\bar{1}\ 0\ 1)$ plane in which the dislocation eventually glides. Hence, in our opinion, the overall behaviour of the $1/2[1\ 1\ 1]$ screw dislocation under the effect of an applied stress is principally the same for the two distinct core structures and, therefore, it is not a determining factor in the plastic behaviour of different materials. However, the effect of the displacements perpendicular to the Burgers vector, which can be significant within the core and rather different in degenerate and non-degenerate cores, may play an important role and be significantly different for the two types of the non-planar cores [38].

The next step in studies of the glide of $1/2[1\ 1\ 1]$ screw dislocations that links the theory with experiment is investigation of the dislocation motion at finite temperatures. This occurs via formation and propagation of kink pairs and while the possibility of investigating this process using the molecular dynamics exists, the development of mesoscopic models may be more fruitful. This will be briefly discussed towards the end of this paper.

2.3. Dislocations with non-planar cores in other materials

It had been known well before the cores of dislocations in BCC metals were studied that dislocations need not be confined to a single crystallographic plane. Examples are the Lomer–Cottrell and Hirth locks [16] in FCC metals. However, the significance of the non-planarity of screws in BCC metals was an important impetus for considering this phenomenon in other materials, in particular when their plastic behaviour did show strong deviations from that known in close-packed structures. This topic

was recently reviewed in the series Dislocations in Solids [18] and we only highlight here a couple of cases to which computer modelling contributed very significantly.

One such case is intermetallic compounds with the $L1_2$ structure, some of which, in particular Ni_3Al , display so called anomalous increase of the yield stress with increasing temperature that is accompanied by the orientation dependence of the yield stress, tension–compression asymmetry and associated breakdown of the Schmid law. It is now generally recognised that this behaviour results from transformations of the $1/2\langle 1\ 1\ 0 \rangle$ screw superpartials from the planar to non-planar configuration as the temperature increases. The non-planar configuration, akin to Kear–Wilsdorf locks [39], was identified by computer modelling in those $L1_2$ compounds in which the complex stacking fault (CSF) on $\{1\ 1\ 1\}$ planes is metastable (for a review see [40]). A detailed theory of the anomalous increase of the yield stress, including the orientation dependencies, was developed on this basis [41]. However, the $L1_2$ structure is an example of the crystal structure in which the stability of the CSF is not guaranteed by symmetry even though this structure is based on FCC lattice. Hence, there may be $L1_2$ compounds in which this fault is unstable. Such possibility was studied by computer modelling [42] and it was found that in this case $1/2\langle 1\ 1\ 0 \rangle$ screw superpartials have only non-planar cores, spread into two different $\{1\ 1\ 1\}$ planes. This situation is completely analogous to $1/2\langle 1\ 1\ 1 \rangle$ screw dislocations in BCC metals with the yield stress increasing with decreasing temperature while no anomalous increase of the yield stress occurs. Such behaviour was observed, for example, in Pt_3Al [43]. Hence, the possibility of alternate core structures of the $1/2\langle 1\ 1\ 0 \rangle$ superpartials, identified by computer modelling, suggests that there are two types of $L1_2$ compounds with distinctly different temperature and orientation dependencies of the yield stress.

Another interesting case, studied recently, is $TiAl$ that crystallises in the FCC based $L1_0$ structure. The calculations of γ -surfaces for $\{1\ 1\ 1\}$ planes, made using a density functional theory method, suggest either a very high energy or an unstable CSF [44]. Consequently, the ordinary $1/2\langle 1\ 1\ 0 \rangle$ screw dislocation does not dissociate into Shockley partials and it was found in atomistic studies employing a bond-order potential for $TiAl$ [45] that its core was non-planar but spread into two $\{1\ 1\ 1\}$ plane and its Peierls stress is of the same order of magnitude as that of screw dislocations in BCC metals [46,47]. Moreover, atomistic studies of the motion of these dislocations near some lamellar interfaces (120° rotational fault and/or a pseudo-twin) showed that the ordinary $1/2\langle 1\ 1\ 0 \rangle$ superpartial may dissociate into Shockley partials and its core becomes planar because the CSF energy is much lower at the interface than in the bulk [48,49]. This finding may provide an explanation for the higher ductility of lamellar structures than single phase $TiAl$ and for the so-called channelled flow [50].

As discussed in detail in the review [18], dislocations with non-planar cores are found in hexagonal crystals when the slip is on other than basal planes, intermetallics with $B2$, DO_{19} and DO_{22} structure, $MoSi_2$ with a body-centred-tetragonal $C11_b$ structure, ionic crystals including perovskites and geological materials like olivine, as well as in molecular crystals. An important phenomenon, discussed above for intermetallics of the $L1_2$ type, is transformations between planar and non-planar cores that may control the most important aspects of the deformation. Another example, revealed by atomistic studies employing a bond-order potential for iridium [51], is the possible transformation between planar and non-planar dislocation core that may explain the brittleness of iridium even though an extensive plastic deformation takes place [52,53]. Hence, the atomistic modelling of dislocation cores in various materials demonstrates that non-planar cores are a ubiquitous phenomenon while planar cores of the type found in FCC metals are a special case. Consequently, as pointed out by Sir Alan Cottrell at the meeting to celebrate the fiftieth anniversary of dislocations [54], the paradigm commonly based on dislocation properties and behaviour in FCC metals needs to be reconsidered.

2.4. Relation of core effects to the macroscopic plastic behaviour

The modelling discussed in the previous sections are all studies of the structure and glide of dislocations at 0 K, obtained using molecular statics calculations. On the other hand, it is the temperature and strain rate dependence of the yield or flow stress that is of interest on mesoscopic and macroscopic levels. Hence, on the dislocation level we need to find the velocity of moving dislocations as a function of the applied stress and temperature and how it relates to the dislocation core properties found on the atomistic scale. A seemingly straightforward approach would be a molecular dynamics

study of a dislocation subject to an applied stress at a finite temperature. Such calculations were attempted [55,56] and they prove that the generally assumed mode of the motion of $1/2[1\ 1\ 1]$ screw dislocations in BCC metals is, indeed, formation and subsequent extension of pairs of kinks. However, at temperatures well below the melting temperature, such calculations could only be made for unrealistically high applied stresses and related very high strain rates owing to the time period that can be realistically studied by molecular dynamics. Moreover, to investigate complex orientation dependencies related to the twinning–antitwining asymmetry and to the dependence on the shear stress perpendicular to the Burgers vector, such calculations would have to be repeated many times over for various types of loading.

A different approach is to employ the theory of thermally activated motion of dislocations based on the reaction rate theory that had been employed in many different mechanisms of dislocation glide [57,58]. In this case the main task is to determine the corresponding activation enthalpy as a function of the applied stress tensor. Several mesoscopic models employing the notion of formation of kink pairs were developed. The models most appropriate for BCC metals are Seeger's theory [59] of kink repulsion applicable at low stresses and the line tension based theory of Dorn and Rajnak [60] for intermediate and high stresses. However, the latter model requires knowledge of the Peierls barrier that is not determined in molecular statics calculations. Furthermore, if the above mentioned effects of the orientation of loading are to be correctly included the Peierls barrier has to be regarded as intrinsically dependent on the applied stress. This feature of the Peierls barrier has been recognised only recently [61,62], whilst all the previous studies assumed that the Peierls barrier is stress independent, determined just by the lattice structure and particular interatomic bonding. A possible approach for determining the barrier is application of the nudged elastic band method (see e. g. [62,63]) but the problem is again the need for a vast number of expensive calculations needed to determine the dependence of the Peierls barrier on details of loading.

An alternative, albeit approximate approach is to use extensive data on the dependence of the Peierls stress on the applied stress tensor obtained in molecular statics calculations performed at 0 K. The Peierls barrier is constructed such that it obeys the symmetry of the corresponding slip plane, similarly as in [64], and its maximum derivative reproduces the Peierls stress. The magnitude of the barrier cannot be determined in this way but it can be fitted to other data, such as those obtained by the nudge elastic band model calculations for a limited number of stress applications and/or by reproducing the experimentally observed yield stress at one temperature. This approach was developed in [61] and an excellent agreement with experimental observations of both orientation and temperature dependencies of the yield stress of molybdenum was attained. In this way the stress and temperature dependence of the velocity of screw dislocations is obtained that can be used in the dislocation dynamics calculations. Alternatively, using the Orowan relation between the strain rate and the velocity and density of mobile dislocations [58], the flow criterion relating the applied stress tensor (not just the shear stress in the direction of the Burgers vector) to temperature and strain rate can be formulated [65]. This criterion may then be used in continuum studies of non-associated flow [66–68], i. e. when shear stress parallel to the slip direction does the work during deformation but other components of the applied stress tensor affect the magnitude of the shear stress needed for yielding to take place.

3. Thoughts about present state and future development

While the beginning of atomistic computer modelling of materials dates to fifties and sixties of the last milenium, a rapid advancement took place in the last two decades so that computer modelling has become equally essential part of materials science as experiments and it is becoming a vital part of education even on the undergraduate level [69]. It is by no means limited only to the mechanical behaviour that is the topic of the main part of this contribution. Computer modelling now encompasses virtually all aspects of materials science: Examples are investigation of stable and metastable structures of complex alloys and related phase diagrams (CALPHAD), interfaces and surfaces including interfacial chemical reactions [70], nano-particles and generally structures and properties on nano-scale [71], amorphous materials [72], radiation damage of materials [73], etc. It is not limited to met-

als, as it was in the early stages, but includes all types of hard materials as well as polymers and other soft materials, including biological substances. Moreover, many modern experimental techniques are completely intertwined with the computer modelling. An example is the electron microscopy of lattice defects, in particular the high resolution electron microscopy, as reviewed, for example, in [74].

Empirical potentials, such as pair potentials, EAM and Finnis–Sinclair potentials, which have been employed in the majority of atomistic studies of crystal defects, are fitted to certain equilibrium properties of specific materials but do not reflect reliably the electronic nature of bonding. On the other hand, the DFT allows us to take fully into account the electronic structure of the material studied and thus include correctly the quantum mechanical aspects of bonding for metals, ionic crystals, covalently bonded solids and, importantly, also for materials with mixed metallic and covalent bonding, such as transition metals. Hence, the important results obtained using empirical potentials are valuable if they reveal certain generic features common to a whole class of materials but less important and reliable if they relate to a specific material. An example of the former is the non-existence of metastable stacking faults and related non-planar structure of the core of screw dislocations in BCC metals. In contrast, the DFT based calculations provide a tool for atomic level studies of specific materials even when their bonding character is complex and none of the common empirical potentials is appropriate.

However, there are two large limitations on the use of DFT methods when studying extended crystal defects. First, the employed atomic blocks can only be relatively small; blocks composed of one thousand particles are usually over the limit of available codes. Hence, if using a finite cluster of particles the free surfaces become a very significant part of the study. Of course, most DFT calculations employ periodic boundary conditions but in this case it is necessary to investigate periodic arrays of defects, for example, dipoles or quadrupoles of dislocations. Owing to the block size these defects may be so close to each other that their interaction dominates the results of calculations. Hence, in spite of the availability of the DFT methods, it is essential to advance further descriptions of atomic interactions that are usable for much larger blocks of atoms, do not require periodic boundary conditions and reflect as closely as possible the essential quantum mechanical aspects of bonding in specific materials. In the development of such potentials the DFT provides invaluable data bases that would never be available empirically and thus the combination of DFT calculations with the development of appropriate semi-empirical schemes is most profitable. Examples are the recent bond-order potentials [75] and potentials based on generalised pseudopotential theory [14] for transition metals and alloys with mixed covalent and nearly free electron type bonding.

Discussing the future is always a very uncertain and even dubious task. In fact, if a real breakthrough occurs in the future it is definitely unpredictable. Notwithstanding, at present it can be expected that atomistic modelling of material structures and properties will be advancing along the same path as in recent years. We cannot expect that atomistic modelling of its own will lead to solving all the important problems of materials behaviour. However, its link with mesoscopic and even macroscopic models and with experimental studies is likely to lead to qualitative steps forward. An example of such link is the connection between atomic level study of screw dislocations in BCC metals and mesoscopic development of rate equations for dislocation motion leading to macroscopic flow criteria. Excellent mesoscopic theories have been advanced in the past that can benefit immensely from links with recent atomistic studies and they often need to be resurrected. This is certainly one fruitful avenue of the development in future. Linked with this advancement is development of new schemes for description of atomic interactions that reflect as closely as possible the quantum mechanical character of bonding, often introduced via DFT studies, and at the same time allowing very extensive calculations preferably without the use of periodic boundary conditions. One such development is analytical bond-order potentials that can be employed in both metallic and covalent materials [76].

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