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An energetic study on the preference of the habit plane in fcc/bcc system

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Abstract. The preference of the habit planes (HPs) developed from precipitation in the fcc/bcc system has been investigated. The interfacial energy of different interface orientations has been examined with variation of the orientation relationships (OR) and lattice parameters by a classical molecular dynamics method. The results show that interface has the lowest interfacial energy when it contains parallel Burgers vectors and a set of dislocations. The local minimum of interfacial energy may not associated with a maximum of dislocation spacing. It is also found that the near Kurdjumov-Sachs OR is more preferable than the near Nishiyama-Wasserman OR. Contrary to the previous interfacial energy calculations, which usually limit to rational ORs, the present work allows ORs to be irrational, which agrees with the observations.

Introduction

The habit planes (HPs) of precipitates are a basic feature in the microstructure generated from precipitation processes. Knowledge of the preference of the HPs is essential to understanding the formation and evolution of the microstrucutre and corresponding mechanical properties. The HPs in different alloys in the fcc/bcc system have been studied in numerous investigations [1-7]. Their oreintations are irrational, and they are often approximately expressed with high indexes, such as $\{335\}_f$ [3]. The preference of these irrationally-oriented HPs have been interpreted by a number of models, such as structural ledge model [8, 9], invariant line model [2, 10], Burgers vector content method [11], O-line criterion [12, 13], near coincidence site (NCS) method [9, 14], and Edge-to-Edge matching method [15], etc., as reviewed in [16]. These models are based on a description of geometric matching, which presumably provides an indication of the interfacial energy. However, the limitation of geometric criterion has impeded differentiation among a set of interfaces that all satisfy a selected geometric criterion. Moreover, no phycial property of the lattices, such as elastic constant, is invovled in the models. Several energy parameters have been proposed to represent the interfacial energy in terms of the dislocations in the interfaces, such as P parameter [17], R parameter [18, 19], and F parameter [11]. However, the dislocation structures in the interfaces for these energy parameters were based on an oversimplied dislocation model. The contribution of the dislocation cores was either neglected or simplified. More recently, the interfacial energy for some simple systems has been evaluated by employing the atomic potentials, such as studies in pure iron [20-22] and Ni-Cr alloy [23]. The OR and HP was usually taken as an input for such a study. A rational OR, such as exact N-W OR [20, 21] or K-S OR [22, 23], is assumed in these studies. However, the experimental results often shows that the observed OR actually deviates from a rational one [3-5].

In this work, the interfacial energy of the irrational HP in the fcc/bcc system have been studied for understanding why a particular irrational HP is preferred. It would be an enormous task to identify the low energy interfaces according to variation of the interfacial energy, since there are five degrees of freedom to describe an interface, i.e. three for the OR and two for the HP normal. To make efficient calculations, we have applied the structure singularity condition to confine the possible geometry of the preferred OR and HP orientation in 5-D space as the first step. Then, the interfacial energy is calculated by an atomic method to further narrow the possible preferred OR and HP.

Geometrical and Energetic Methods

Geometrical Method. The correspondence between singularity (local minimum) in the interfacial energy and that in the interfacial structure has been suggested for identifying the candidates of singular interface [24]. For example, an interface that is free of any interfacial defects of either dislocations or ledges is expected to be a singular interface corresponding to a local energy minimum. Accordingly, one can search for the OR and HP normal that allow present of the defect free structure. However, such defect free structure is only possible when the lattice parameters of the two lattices are specially related. In a general system, dislocations must be present in an interface of any orientation at any OR. Then, a possible singular interface will contain at least a single set of dislocations. When a dislocation free interface is unavailable, an interface containing a set of dislocations is a singular interface, because any deviation in the interface orientation will cause introduce of a new type of dislocation and hence an increase of interfacial energy. In addition, an arbitrary deviation in the OR will also destroy the single set dislocation configuration. This single set dislocation condition is equivalent to the O-line criterion [12], which is supported by the observations from many systems [13]. However, the O-line criterion only restricts two of three degrees of freedom in the OR [16, 25], thus there are many ORs and corresponding HPs meeting the O-line criterion. For fcc/bcc system, the analytical solutions for these ORs and HPs have been derived as functions of lattice parameter ratio (LPR = a_f/a_b) and the angle between the Burgers vectors $\mathbf{b}^L = [1\,\bar{1}\,0]_f/2 \mid [100]_b$ or $[\bar{1}\,01]_f/2 \mid [\bar{1}\,\bar{1}\,1]_b/2$ [25]. According to these analytical formulas, a series of HPs and ORs together with the direction and spacing of the interfacial dislocation can be obtained for a given alloy in fcc/bcc system. Since there are many HPs that all satisfy the O-line criterion, an energetic study must be carried out to find the preferred interface. The NCS percentage [14] is useful to indicate the degree of good atomic matching. A NCS is defined when atomic misfit is smaller than 15%$|\mathbf{b}_f^L|$, where $\mathbf{b}_f^L$ is the Burgers vector in fcc. This parameter will be determined for a comparison with the energetic calculations.

Energetic Method. In contrast to the rigid geometrical model, the relaxed interfacial structures and the interfacial energy can be calculated by employing atomic potentials. The Morse potential and embedded atom method (EAM) potential [26] are applied for modeling the interaction between the atoms. For specific alloys, the parameters for EAM potential are adopted from the literatures. These potential can incorporate many body nature of the interaction between atoms. However, it is meaningless to fit a series of EAM potentials for some hypothesized alloys in order to study the variation of the interfacial energy with the LPR, because a lot of uncertainties are involved in the fitting process and it is not trivial to fit a good EAM potential. Therefore, Morse pair potential is employed in this work to study the interfacial energy with variation of the LPRs. The parameters for this potential can be simply determined and the advantage of its simple form outweighs its well known disadvantages in this application. It is also found that the pair potential can reproduce the relaxed interfacial structures calculated by EAM potential. The parameters of the Morse potentials for fcc and bcc lattices are fitted according to the properties (lattice parameter, cohesive energy and bulk modulus) of the pure alloy iron and copper from Ref. [28]. The parameters for the potential between two dissimilar atoms, i.e. iron (bcc) and copper (fcc), are determined from mixing rules in Ref. [27]. By only changing the lattice parameter of one bcc lattice, one can fit series Morse potentials for different LPR.

The atomic configurations between the rigid fcc and bcc lattices are set up after the OR and HP being determined from the O-line method [25]. At the beginning, the blocks of fcc and bcc lattices are oriented at an OR and separated by a HP determined from this method. Then, the system is relaxed by two steps with fixed boundary conditions. Firstly, the fcc lattice and bcc lattice are rigidly translated to each other to find the minimum energy configuration. Then, the system is dynamic relaxed at 300k until the global energy is minimized. Finally, the system is quenched to 0 k and static relaxed. All of these calculations are performed by using the parallel atomistic simulation code LAMMPS [30]. Finally, the interfacial energy between fcc and bcc are determined as the excess energy per unit area

by comparing with the perfect crystals. The sample box is selected with each face kept at least 1 nm from the fixed boundary and the sample area parallel to HP is taken as the multiple size of the O-lattice cell to minimize the error. In general, each side of the box is ranged from 5nm to 10nm.

Results

Take a Fe-Cu alloy system for example, the interatomic potential is adopted from Ref. [29], and the ORs and HPs is calculated from the formulas with LPR = 1.2611 in [25]. Fig. 1(a) and 1(b) shows the variation of the interfacial energy for the interface containing O-line with $\mathbf{b}^L$ as $[1\,\bar{1}\,0]_f/2 \mid [100]_b$ and $[\bar{1}\,01]_f/2 \mid [\bar{1}\,\bar{1}\,1]_b/2$ respectively. The interfacial energy varies significantly, and the lowest interfacial energy is achieved when the Burgers vectors are parallel to each other, i.e. $[1\,\bar{1}\,0]_f/2$ // $[100]_b$ (namely, Type I OR in [13]) or $[\bar{1}\,01]_f/2$ // $[\bar{1}\,\bar{1}\,1]_b/2$ (named Type III OR in [13]). The Type I OR is near N-W OR with the angle between $(111)_f$ and $(011)_b$ being about 0.44° and the HP is $(1\ 1\ 1.70)_f$//$(0\ 1\ 1.70)_b$. The direction and spacing of dislocations in the HP are $[1\ 1\ \overline{1.18}]_f$ // $[0\ 2\ \overline{1.18}]_b$ and 2.36 nm respectively. The Type III OR is near K-S OR with the angle between $(111)_f$ and $(011)_b$ being about 0.48° and the HP is $(1\ 1.79\ 1)_f$//$(\bar{1}\ 3.55\ 2.55)_b$. The direction and spacing of dislocation in the HP are $[1\ \overline{0.09}\ \overline{0.84}]_f$ // $[1\ 0.83\ \overline{0.77}]_b$ and 0.972 nm respectively. The variations of NCS percentage and the dislocation spacing in the HP are also shown in Fig. 1. For all of the interfaces, the percentage of NCS is virtually the same and is about 20% ~ 30% in consistence with up limit theoretical value 30% [7], though the interfacial energy varies. Notice that the minimum interfacial energy corresponds to a maximum of dislocation spacing for $\mathbf{b}^L = [1\,\bar{1}\,0]_f/2 \mid [100]_b$ in Fig. 1(a). However, it is not the case for $\mathbf{b}^L = [\bar{1}\,01]_f/2 \mid [\bar{1}\,\bar{1}\,1]_b/2$ in Fig. 1(b). It is recognized that the interfacial energy corresponding to the HP with the maximum dislocation spacing carries relatively large uncertainty due to complex atomic structure in the interface.

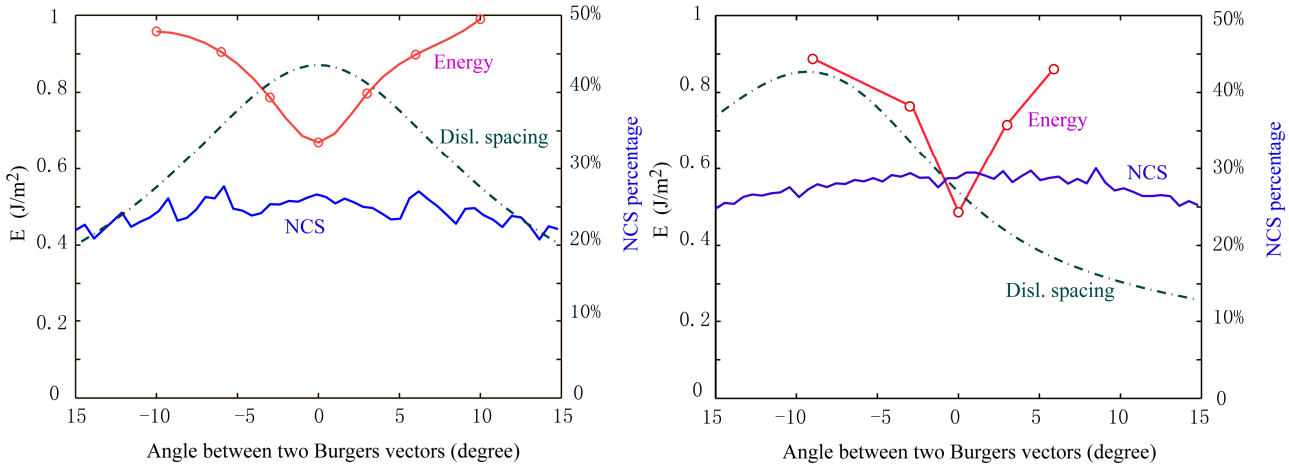

Fig. 1 Variation of the interfacial energy, NCS percentage and dislocation spacing in the interface satisfying O-line condition with Burgers vectors as (a) $[1\,\bar{1}\,0]_f/2 \mid [100]_b$ and (b) $[\bar{1}\,01]_f/2 \mid [\bar{1}\,\bar{1}\,1]_b/2$ in a Fe-Cu system.

Figure 2 shows the relaxed atomic configurations for the interface with O-lines for Fe-Cu at Type I OR. Fig. 2(a) shows the atomic configuration near the interface $(1\ 1\ 1.70)_f$ // $(0\ 1\ 1.7)_b$. One set of dislocations is indicated by the atoms with higher energy with unfavorable stacking sequences, i.e. "AA" for both fcc and bcc lattices. The regions between the dislocations are fully coherent. The atomic plane from one lattice in the coherent region approximately repeats the stacking sequence of the atomic plane from other lattice. Fig. 2(b) is side view of the relaxed atomic configuration from an edge-on view along $[1\,\bar{1}\,0]_f$// $[100]_b$. One can see that the atomic planes from one side of the interface run continuously across the interface to the other lattice. However, the interface is not coherent as shown in Fig. 2(a), because the misfit displacement is along the zone axis in Fig. 2(b).

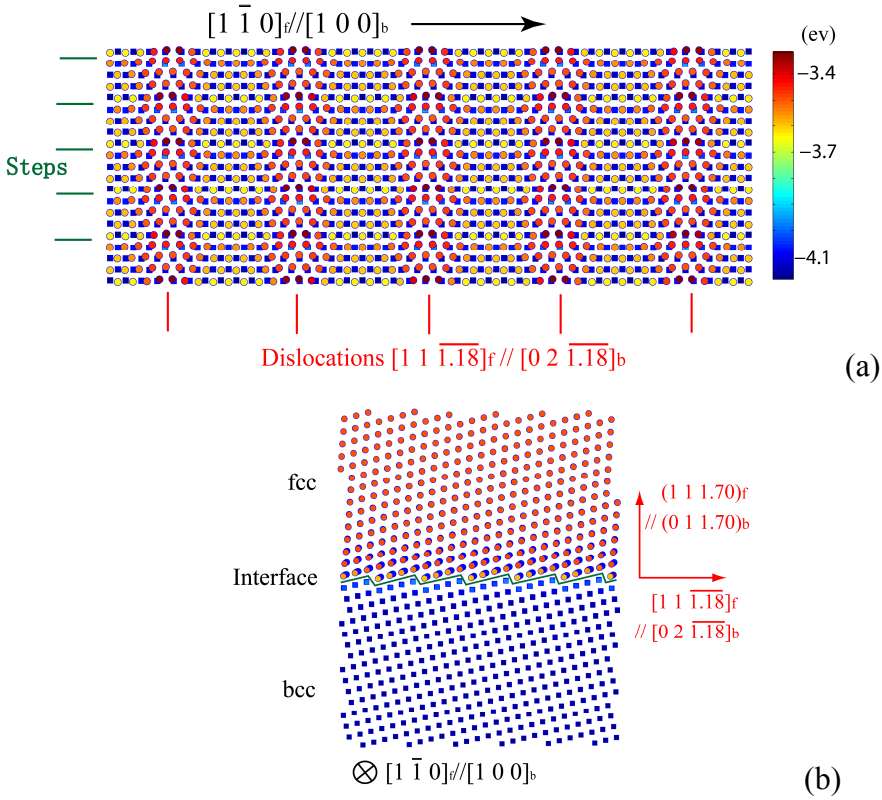

Fig. 2 (a) Relaxed atomic structures around the interface viewed along the HP normal and (b) atomic configurations viewed along the parallel directions $[1\,\bar{1}\,0]_f$// $[100]_b$. Atoms are colored according to their cohesive energy.

The interfacial energy for all interfaces containing the parallel Burgers vectors at Type I OR and Type III OR for Fe-Cu alloy are also calculated as shown in Fig. 3(a) and 3(b) respectively. The interfaces surrounding the secondary phase are mainly consist of the interface containing the O-line and $(111)_f$. It is also found that the minimum interfacial energy are reached when the interface contains the O-line, which is about -15° and -16.3° from the $(111)_f$ plane for Type I and Type III OR respectively. The NCS percentage has also been calculated and plotted in Fig. 3. One can see that the peak of NCS corresponds to the minimum interfacial energy for base cases. The result indicates that the interface containing O-line and the parallel Burgers vectors is a singular interface other than those only containing parallel directions.

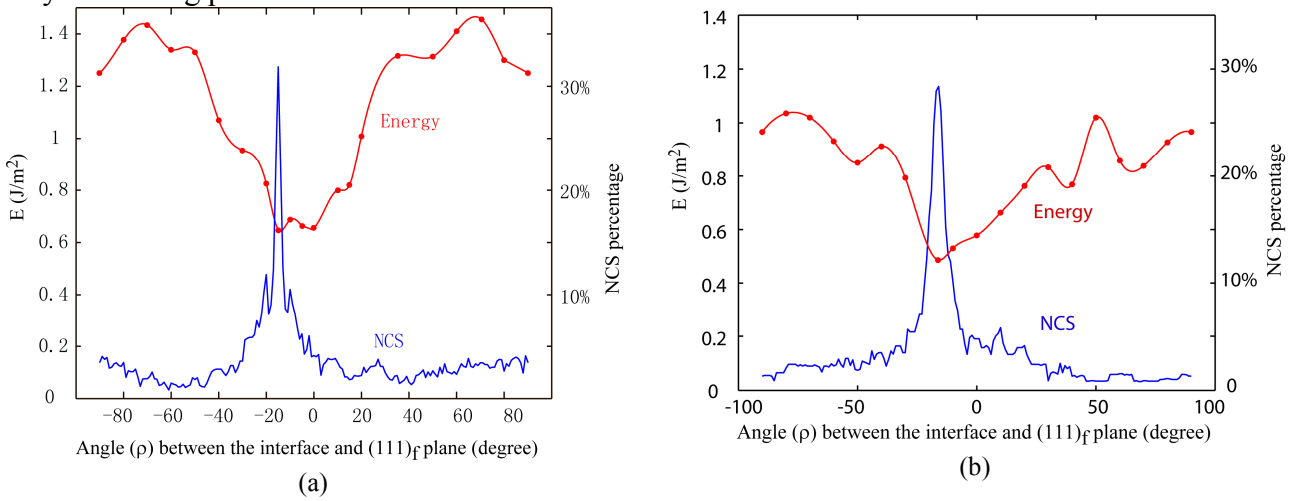

Fig. 3 The interfacial energy and NCS percentage for an Fe-Cu alloy with series interfaces containing (a) $[1\,\bar{1}\,0]_f$// $[100]_b$ at a Type I OR and (b) $[\bar{1}\,01]_f$// $[\bar{1}\;\bar{1}\;1]_b$ at Type III OR. The inserted figures are the morphology of the secondary phase determined by the interfacial energy.

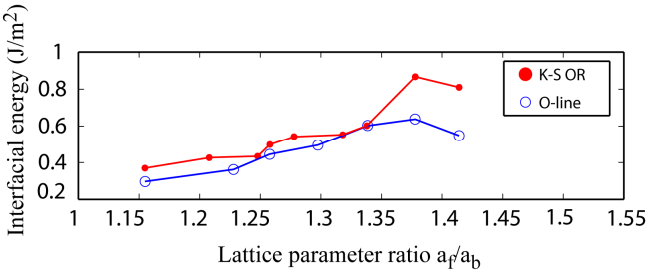

Fig. 4 The variation of the interfacial energy with LPR at the exact K-S OR (solid dots) and the OR at Type III OR (open dots).

As mentioned earlier, a singular interfaces tends to be free of any defects, including steps and dislocations. The step free interface $(111)_f$ // $(011)_b$ at the exact K-S OR is compared with the HP containing O-line at Type III OR. Fig. 4 shows the variation of the energies with LPR for these two cases. It is shown that the interfaces containing the O-line always have lower interfacial energy. Note that when LPR = 1.33, the HP at Type III OR is $(111)_f$ // $(011)_b$ [25], and the energies coincide.

Since the interface containing the O-line and parallel Burgers vector directions is preferred, the interfacial energy for the HP containing different parallel Burgers vectors and the O-line were compared in several alloy systems as shown in Table 1. It is found that the interfacial energy at a near K-S OR (Type III OR) is always lower than that at the near N-W OR (Type I OR). It explains why the near K-S OR is often observed [2-3]. According to the O-line model [25], the dislocation spacing for near N-W OR is about 2.5 nm while the dislocation spacing for the near K-S OR is about 1 nm when LPR is near 1.25. Hence, the preference of these two ORs purely according to the dislocation spacing may be misleading. This may be understood in terms of dislocation core. When the dislocation spacing is mall, the role of dislocation core energy becomes important. The dislocation for Type I OR is of pure edge type, while that for Type III OR is near screw type. The core of later is less distorted comparing with the pure edge type [31].

Table 1 The interfacial energy of the HP at Type I OR and the near K-S OR

Alloy	LPR	Near N-W OR (Type I) [J/m^2]	Near K-S OR (Type III)[J/m^2]	Potentials from
Pure Fe	1.2555	0.387	0.2474	[20]
Fe-Cu	1.2611	0.670	0.486	[29]
Ni-Cr	1.2650	0.485	0.284	[23]

Summary

The preference of the OR and HP in fcc/bcc system has been investigated with a combination of geometric method and energetic method. The geometric method greatly reduced the energetic calculations to these interface containing O-line. According to the energetic studies, it was found the interface with the lowest interfacial energy contains the parallel Burgers vectors. For a given Burgers vector, the local minimum of the interfacial energy may correspond to a local maximum of the dislocation spacing or may not. The relaxed atomic structures corresponding to the HP with minimum interfacial energy are also shown with one set of dilocations, which is in agreement with geometical

assumptions. The interfacial energy of the general interfaces containing parallel Burgers vectors is also investigated. It is also found the interface, containing the O-line and parallel Burgers vectors, is more preferable than those only containing parallel directions. This conclusion is further confirmed by comparing the $(111)_f$ // $(011)_b$ at the exact K-S OR with the O-line interfaces when LPR changes. Energetic study further shows that the interface at near K-S OR has lower interfacial energy comparing with that of N-W OR, though the dislocation spacing is smaller.

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References

[1] J.M. Rigsbee, and H.I. Aaronson: Acta Metall. Vol. 27 (1979), p. 365

[2] C.P. Luo, and G.C. Weatherly: Acta Metall. Vol. 35 (1987), p. 1963

[3] C.P. Luo, U. Dahmen, and K.H. Westmacott: Acta Metall. Mater. Vol. 42 (1994), p. 1923

[4] T. Fujii, T. Mori, and M. Kato, Acta Metall. Mater., 40 (1992), p. 3413.

[5] T. Fujii, H. Nakazawa, M. Kato, and U. Dahmen, Acta Mater., 48 (2000), p. 1033.

[6] H. Jiao, M. Aindow, and R.C. Pond: Philos. Mag. Vol. 83 (2003), p. 1867

[7] D. Qiu, and W.-Z. Zhang: Acta Mater. Vol. 55 (2007), p. 6754

[8] M.G. Hall, H.I. Aaronson, and K.R. Kinsma: Surf. Sci. Vol. 31 (1972), p. 257

[9] J.M. Rigsbee, and H.I. Aaronson: Acta Metall. Vol. 27 (1979), p. 351

[10] U. Dahmen: Acta Metall. Vol. 30 (1982), p. 63

[11] K.M. Knowles, and D.A. Smith: Acta Crystal. A, 38 (1982), p. 34

[12] G. C. Weatherly, and W.-Z. Zhang, Metall. Mater. Trans. A, 25 (1994), p. 1865

[13] D. Qiu, and W.-Z. Zhang: Philos. Mag., 83 (2003), p. 3093

[14] Q. Liang, and W. T. Reynolds, Jr.: Metall. Mater. Trans. A Vol. 29 (1998), p. 2059

[15] P. M. Kelly, and M.-X. Zhang: Mater. Forum Vol. 23 (1999), p.41

[16] W.-Z. Zhang, and G.C. Weatherly: Prog. Mater. Sci. Vol. 50 (2005), p. 181

[17] W. Bollmann, and H.U. Nissen: Acta Crystal. A Vol. 24 (1968), p. 546

[18] R.C. Ecob, and B. Ralph: Proc. Natl. Acad. Sci. USA Vol. 77 (1980), p. 1749

[19] K.M. Knowles, D.A. Smith, and W.A.T. Clark: Scripta Metall. Vol. 16 (1982), p. 413

[20] Z. Yang, and R.A. Johnson: Model. Simul. Mater. Sci. Eng. Vol. 1 (1993), p. 707

[21] T. Nagano, and M. Enomoto: Metall. Mater. Trans. A Vol. 37 (2006), p. 929

[22] J. Chen, D Farkas, and W. Reynolds, in: Proceeding of Solid-to-Solid Phase Transformations, edited by Johnson, W. C., J. M. Howe, D. E. Laughlin and W. A. Soffa., (1994), p. 1097

[23] J. K. Chen, D. Farkas, and W. T. Reynolds, Jr.: Acta Mater. Vol. 45 (1997), p.4415

[24] W.-Z. Zhang, and Z.-Z. Shi: in this symposium (2010)

[25] X.-F. Gu, and W.-Z. Zhang: Philos. Mag. Vol. 90 (2010), p.4503

[26] M.S. Daw, and M.I. Baskes: Phys. Rev. B Vol. 29 (1984), p. 6443

[27] S.K. Das, D. Roy, and S. Sengupta: J. Phys. F: Met. Phys. Vol. 7 (1977), p. 5

[28] C. Kittel: *Introduction to solid state physics* (Wiley, New York, 1996).

[29] G.J. Ackland, D.J. Bacon, A.F. Calder, and T. Harry: Philos. Mag. Vol. 75 (1997), p. 713

[30] S.J. Plimpton: J. Comput. Phys. 117 (1995), p. 1

[31] G. Lu, and E. Kaxiras, Phys. Rev. Lett., 89 (2002), p.105501

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