

Threshold displacement energy in Ni, Al and B2 NiAl

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Abstract. For simulation of radiation effects and defects in the Ni-Al system, a new many body potential was developed by joining the equilibrium part of the Mishin's EAM potential with the universal function of Ziegler, Biersack and Littmark at a suitable interatomic spacing and the corresponding pairwise energy from the DFT calculations. To assess the qualities of this potential, we performed molecular dynamics simulations to calculate the threshold displacement energy of pure metals Ni, Al and their NiAl B2 phase superalloy at ambient temperature. It was found that the threshold energy of displacement of nickel in nickel is higher than that in the B2 long-range ordered alloy NiAl in contrast to aluminium, which has lower threshold energy than B2 NiAl. The threshold displacement energy ranges between 14 ± 2 eV and 189 ± 2 eV depending on the crystallographic direction. The lowest threshold energy of two fcc metals (14 ± 2 eV for Al and 28 ± 2 eV for Ni) was found in the direction $\langle 101 \rangle$, these values correspond to the mean value in the easiest directions of atomic displacements and they are in good agreement with many reports from the literature.

1. Introduction

The threshold displacement energy (TDE) E_d is the minimum kinetic energy that must be given to an atom in a solid in order to displace it permanently from its lattice site to the defect position. TDE is an important factor, which determines the defect production, particularly, the number of Frenkel pairs in NRT and Kinchin-Pease displacement models of primary radiation damage in a material. It is also often used in binary collision approximation computer codes such as SRIM. In a crystalline solid, the TDE magnitude is a function of the crystallographic direction $E_d(\theta, \phi) = E_d([hkl])$, temperature, applied strain and many other factors. One distinguishes the minimum threshold displacement energy, $E_{d,min} = \min(E_d(\theta, \phi))$, and the average or effective one, $E_{d,ave} = \text{ave}(E_d(\theta, \phi))$, averaged over all lattice directions [1].

The calculation of the threshold displacement energy is not a trivial problem, because the cascade displacement under irradiation is a complex multi-body collision process, as has been shown by various research groups, in which several methods have been used [2, 3, 4]. In the case of Ni, Al and B2 NiAl alloy, many studies, both simulation and experiment, have been conducted to find their threshold displacement energy in several crystallographic directions at different temperatures, however the results are significantly different between these research groups [5]. Discrepancies may come from different method and potential applied. For this reason, we performed several classical molecular dynamics (MD) simulations to investigate the threshold displacement energies of pure fcc metals Ni, Al and their B2 phase NiAl superalloy in some crystallographic directions at ambient



temperature (300 K). The authors of this work would like to provide another perspective to this classical problem of radiation damage.

Table 1. Recommended values of the effective displacement energy for use in displacement calculation [1].

Metal	Lattice(c/a)	$E_{d,min}$ (eV)	E_d (eV)
Al	fcc	16	25
Ti	hcp (1.59)	19	30
V	bcc	-	40
Cr	bcc	28	40
Mn	bcc	-	40
Fe	bcc	20	40
Co	fcc	22	40
Ni	fcc	23	40
Cu	fcc	19	30
Zr	hcp	21	40
Nb	bcc	36	60
Mo	bcc	33	60
Ta	bcc	34	90
W	bcc	40	90
Pb	fcc	14	25
Stainless steel	fcc	-	40

2. Potential for simulation of radiation damage

Many potentials have been developed for the Ni-Al system, including the Finnis–Sinclair potential of Yan and the EAM potentials by Foiles and Daw, Voter and Chen [6]. In this work, to investigate the TDE in Ni, Al and B2 NiAl we chose the embedded-atom-method (EAM) potential developed by Mishin et al, [6]. This potential was developed in 2009 using an empirical fitting method. Within the EAM description, the total energy of atom i is given by:

$$E_i = F_\alpha \left(\sum_{i \neq j} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha\beta}(r_{ij})$$

where r_{ij} is the distance between atoms i and j , $\phi_{\alpha\beta}$ is the pair-wise potential function, ρ_β is the contribution to the electron charge density from atom j of type β at the location of atom i , and F_α is the embedding function that represents the energy required to place atom i of type α into the electron cloud.

However, the Mishin’s potential does not meet the requirements and criteria associated with the simulations of radiation damage. Like the aforementioned potentials based on the EAM formalism, it is too “soft” and not suitable for simulating radiation damage at a very short interatomic distance. At such small atomic separations, the force fields fitted to the equilibrium properties tend to significantly underestimate the potential energy of the colliding dimer [7]. To enable molecular dynamics simulations of high-energy collisions, the Mishin EAM potential was modified following the procedure in the work of Stoller et al [7] that involves the use of *ab initio* calculations to determine the magnitude and spatial dependence of pair interactions at intermediate distances, along with systematic criteria for choosing the joining parameters.

There is no generally accepted procedure for choosing the inner and outer cutoff distances to join the equilibrium region of the potential with the higher energy region [4, 7, 8, 9]. In order to test its effect, some MD runs were performed with different inner and outer cutoffs to the spline used to

connect the many-body term and the universal function of Ziegler, Biersack and Littmark (ZBL potential) [10] to the Mishin potential. The most appropriate cutoffs are presented in table 2.

Table 2. Electron density and pair-wise interaction term cutoffs for the modification of the Mishin potential

Interaction	Ni-Ni	Ni-Al	Al-Al
$r_{\text{inner}}(\text{\AA})$	0.2	1	1.7
$r_{\text{outer}}(\text{\AA})$	2	1.6	2.3
Electron density cutoff (\AA)	1.5		

Modifications are made to the many-body term of the EAM, namely the density and embedding functions. The goal is to have the repulsive pair interaction term of the EAM play the major role in describing the resulting energetics as the distance between two atoms decreases. To ensure this, the embedding energy term has to become negligible by either becoming constant or very small [7]. A spline interpolation was used to create a smooth transition from the original density function at $r = 0.15$ nm to zero at $r = 0$. This modification reduces the contribution of the many-body embedding energy term as the atom closely approaches its neighbor [7].

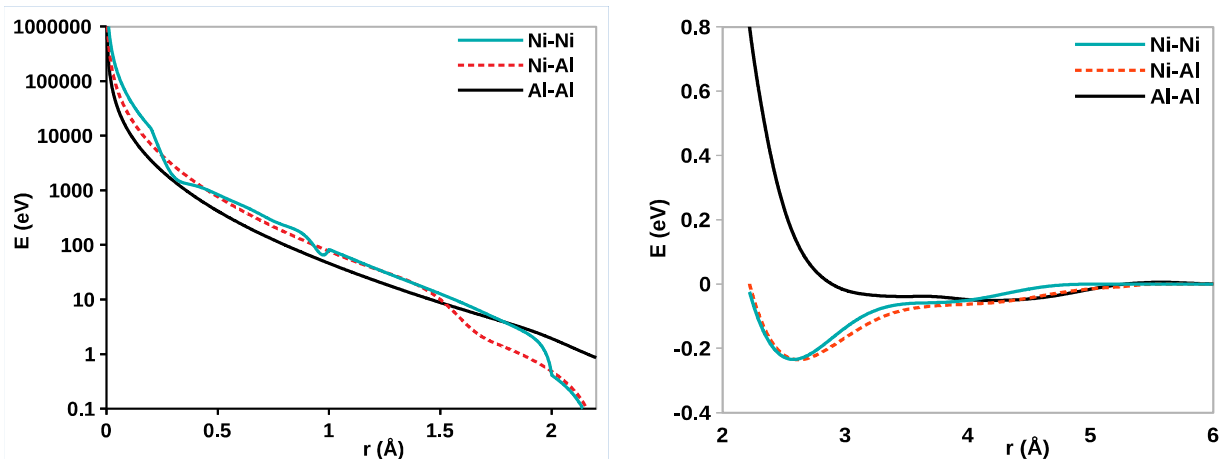


Figure 1. Pair-interaction functions of the modified potential in this study. The right panel is a linear scale plot of the pairwise energy near the equilibrium distance ($r > 2.2$ Å), while the left panel is a log-scale plot of the pairwise energy at a shorter distance ($r < 2.2$ Å).

All two-body terms, pair interaction terms as described in figure 1 need to be modified in two regions: at a very short distance $0 < r < r_{\text{inner}}$ the total energy must match the ZBL potential, at an intermediate distance $r_{\text{inner}} < r < r_{\text{outer}}$ it must match target values for the dimer energy in crystalline Ni-Al obtained from DFT calculations [7]. In the equilibrium region, where $r_{\text{outer}} < r < r_{\text{cutoff}}$ the force field needs to be equal to the original Mishin potential in order to preserve all its equilibrium properties. All regions were joined together using polynomial regression to maintain the continuity of the second derivative at the joining points, particularly when the Verlet method is used to integrate the equations of motion. After that, the *atsim.potential* package [11] was used for the specification and tabulation of pair-terms and many-body terms to EAM setfl file format, which is directly supported by the most popular classical MD code LAMMPS [12].

The modified potential correctly reproduced the equilibrium lattice parameters, cohesive energies, lattice constants and others equilibrium properties of pure Ni, Al and their alloys B2 NiAl, L12 Ni₃Al.

To assess the qualities of this potential in higher energy collision simulation, we performed several classical MD simulations using LAMMPS to calculate the threshold displacement energies of Ni, Al and B2 NiAl in some crystallographic directions at ambient temperature.

3. Threshold displacement energy simulation

The LAMMPS MD with GPU and Voronoi package [12, 13, 14] was used to simulate the displacement cascades in a simulation box containing $30 \times 30 \times 30$ unit cells with periodic boundary conditions that are applied in three directions.

Our simulations were run with a two layer wide Langevin bath at 300 K to evacuate the extra heat. Initially, the temperature was thermostated at 300 K, and the pressure was barostated to zero in 10 ps. After the primary knock-on atom (PKA) was given the first kinetic energy of 100 eV in some of the basic crystallographic directions, the MD run was carried out at a constant NVE. A variable time-step of at least 0.2 ps was used to limit the distance traveled by atoms between time-steps to ensure numerical accuracy and simulation efficiency. After 0.2 ps with a variable time-step for a primary collision, the simulation time-step resets to 0.001 ps and the system is equilibrated for 10 ps. The number of stable Frenkel pairs is calculated by the Voronoi and Wigner-Seitz cell analysis [14, 15, 16]. This process continues with the binary search algorithm until at least one stable Frenkel pair remains after the simulation. For each direction, total 10 simulations were performed to obtain a confident estimate of the average TDE. The average results of the TDE in each direction are presented in table 3.

Table 3. Average values of the TDE in corresponding direction

Direction [hkl]	Threshold displacement energy ($E_d \pm 2$ eV)			
	Ni	Al	Ni in B2 NiAl	Al in B2 NiAl
100	48	14	17	14
010	54	20	17	17
001	45	20	24	20
110	32	14	29	20
101	28	14	17	17
011	28	14	60	39
111	98	24	83	36
1 0.5 0.5	132	45	92	36
0.5 1 0.5	142	39	51	54
0.5 0.5 1	64	54	58	76
135	189	36	101	60
720	45	23	20	45
210	113	33	26	39
211	132	45	92	36
520	72	20	23	39
441	114	14	23	40
322	189	30	92	54
311	130	45	117	23

From the results shown in table 3, it is seen that the threshold energy of nickel in pure metal nickel is higher than its value in the B2 long-range ordered NiAl alloy in contrast to aluminum with the

threshold energy in B2 NiAl larger than its value in pure metal Al. The threshold displacement energy is ranging between 14 ± 2 eV – 189 ± 2 eV, depending on the crystallographic direction. There are no experimental data available for the highest threshold displacement energy $E_{d,max}$ and the threshold displacement energy in the B2 NiAl alloy [2]. The lowest threshold energy $E_{d,min}$ of two fcc metals (14 ± 2 eV for Al and 28 ± 2 eV for Ni) was found in the direction $\langle 101 \rangle$, these values correspond to the mean value in the easiest directions of atomic displacement and they are in good agreement with many reports from the literature [1, 2, 3, 5, 17, 18]. However, our simulations do not provide a consistent value of the effective threshold displacement energy. This is the expected behavior, because the modified potential in this work is an empirical potential, in which the effects of the ion-electron interaction (electronic stopping power) and the electron-phonon interaction were neglected. Moreover, in order to obtain the value of the effective threshold displacement energy, we have to execute sufficiently larger simulations in a sufficiently larger crystallographic direction.

4. Conclusions

To enable molecular dynamics simulation of high energy collisions, a new many body potential was developed by joining the equilibrium part of the Mishin EAM potential for the Ni-Al system with the universal function of Ziegler, Biersack and Littmark at a suitable interatomic spacing and the corresponding pairwise energy from DFT calculation. To assess the qualities of this potential, we performed MD simulations to calculate the threshold displacement energy of pure metal Ni, Al and their NiAl B2 phase superalloy at ambient temperature. Many authors from the literature used the linear search method to calculate the TDE with the time complexity $O(n)$. In this work, we applied the binary search method with the time complexity $O(\log(n))$, a faster approach to simulation of the threshold displacement energy. The simulation results are in good agreement with other data from the literature, sufficient to prove the accuracy of this potential. Therefore, it is suitable for simulating radiation damage with the higher energies collision.

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