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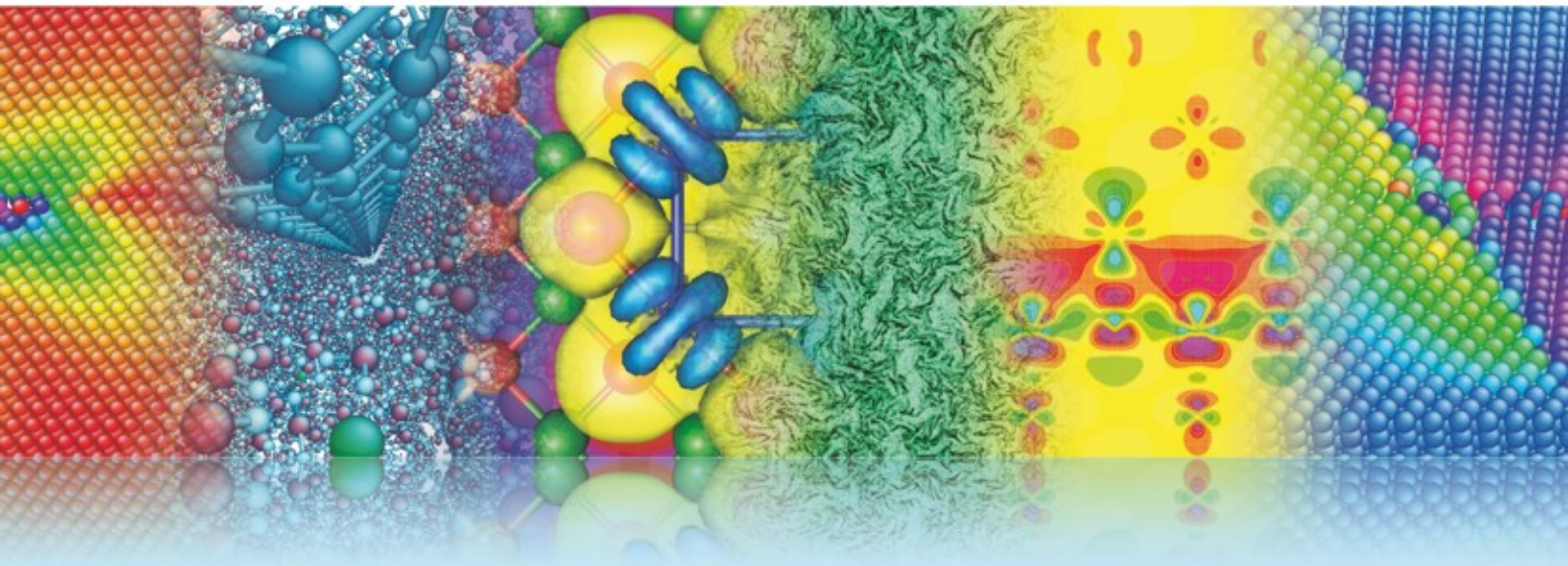

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Reconstruction of dislocations in interface layer Cu-Al_2O_3

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ABSTRACT

Using three different methods namely, CDT (Continuous Dislocation Theory), molecular TB-SMA (Tight Binding Second Moment Approximation) type many-body potential, and MEM (Molecular Effective Medium) theory, we are looking for the best possible reconstruction of dislocations in Cu-Al_2O_3 heterostructure.

1. Introduction

The issue of assessing the strength and functionality of heterostructures metal - ceramic is very important both from a cognitive, as well as from a practical point-of-view.
An important, often decisive factor is knowledge of the limit state in the transitional metal – ceramic layer (interface) .
The subject of our modeling is the mismatch dislocation structure - such as those formed in the case of crystal growth of copper on the surface of sapphire (Al_2O_3).

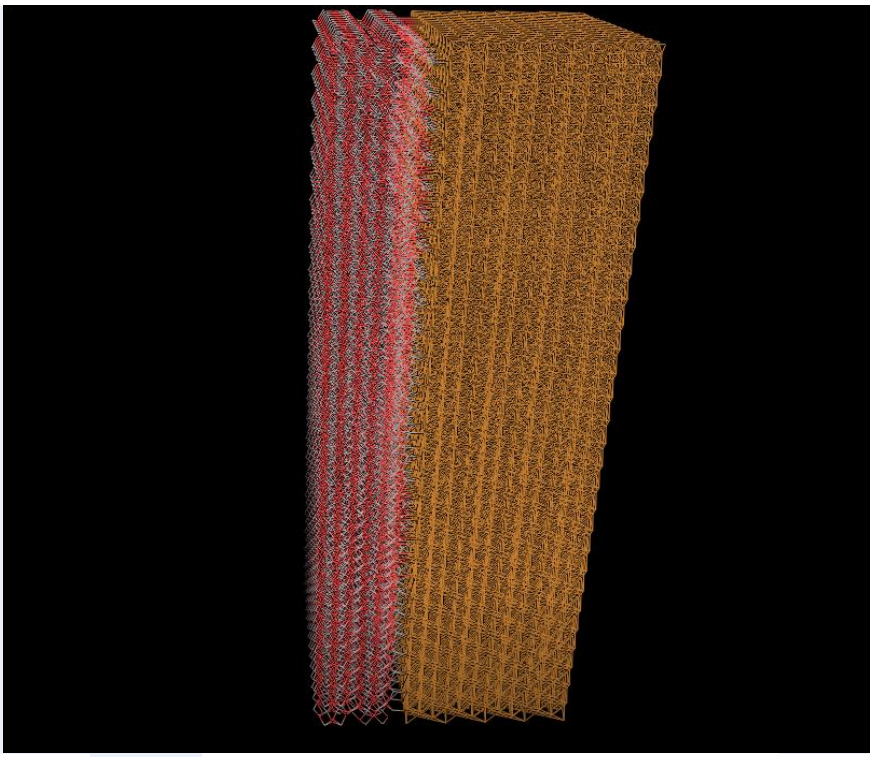

Fig.1. Copper on the surface of sapphire (Al_2O_3)

On the basis of existing experimental research conducted by high-resolution transmission electron microscopy (HRTEM) there is some knowledge available about the system of dislocations resulting from the mismatch between sapphire and copper [1].

We want to reconstruct the system of dislocations in the interface using various methods and compare the results. These methods are:

-Algorithm from Continuous Dislocation Theory based on newly derived analytical models for the insertion of dislocations to the continuum [2,3].

-Atomic method based on the model TB-SMA type many-body potential [1,4,5,6].

- Atomic method based on the original atomic model, in which the interaction occurring inside the layers of the Cu- Al_2O_3 interface will be formulated in accordance with the concept of the method of Effective Medium Theory [7,8].

2. The methods

2.1 Continuous Dislocation Theory - analytical equations for mixed straight dislocation

The displacement field around a mixed straight-line dislocation in an elastic material is defined by the classical formulas [2,3]

$$\begin{aligned} u_x &= \frac{b_x}{2\pi}\left(\arctan\frac{y}{x}+\frac{xy}{2(1-\nu)(x^2+y^2)}\right)-\frac{b_x}{2} \\ u_y &= -\frac{b_x}{2\pi}\left(\frac{1-2\nu}{4(1-\nu)}\ln(x^2+y^2)+\frac{x^2-y^2}{4(1-\nu)(x^2+y^2)}\right) \\ u_z &= \frac{b_z}{2\pi}\arctan\frac{y}{x}-\frac{b_z}{2} \end{aligned} \tag{1}$$

where the edge and screw components of the Burgers vector ,b_x and b_z, are parallel to the *x* and *z* axes, respectively. Using the analytical equations of displacement field induced by discrete dislocations Eqn.1 we introduced dislocations into Cu- Al_2O_3 structure.

2.2. Tight-binding second moment approximation type many-body potential

In the TB-SMA approach [1,4,5,6] potential energy per atom is a sum of the repulsive energy E_{rep}, and the binding energy E_b:

$$E_{rep} = A\sum_i \exp\left(-p\left(\frac{r_i}{r_0}-1\right)\right) \tag{2}$$

$$E_b = -\xi \sqrt{\sum_i \exp\left(-2q\left(\frac{r_i}{r_0} - 1\right)\right)}$$

where r_0 is the distance between nearest neighbours at zero temperature and r_i is the distance of i atom from the considered one, A; p, ξ and q are free parameters.
Parameters are identified by elastic eigen-states approach [8] and differ from the values assumed by Dimitriev [1] but better reproduce energy density of the ideal crystal.

2.3 Potential based on Effective Medium Theory

Using Effective Medium Theory [7] we formulated original embedded-atom method (EAM) potential for Cu-Al_2O_3. The covalent and metallic interactions occurring in the ceramic layer and metal layer are described correspondingly:

$$E_n = \sum_{i=1}^{N} F_i(\rho_i) + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \Phi_{ij}(r_{ij}) \tag{3}$$

The function F_i is the energy of embedding of the i-th atom in the electron density ρ_i and Φ_{ij} is the energy of interaction of pair of atoms. EAM potential can be treated as a more flexible generalization of TB-SMA approach. To parameterize above potential elastic eigen-states approach was used with two kinds of tensile tests: so called relaxed tensile test, the sample cut off from the surroundings of the interface is being stretched in the direction normal to the interface and so called rigid tensile test.

3. Conclusions

We presented three methods of the reconstruction of dislocations in Cu-Al_2O_3 heterostructure. First, the analytical one, where equations of displacement field induced by discrete dislocations are used. Next two utilize molecular approach and respectively are based on tight-binding second moment approximation potential and embedded-atom potential.
Using these methods, a relaxed structure with minimal energy will be further chosen for nanoindentation simulation in which the behaviour of the dislocation structure if nonequilibrium configuration is investigated .

Acknowledgments

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