Atomistic/continuum reconstruction of misfit dislocations and stacking faults in Cu/sapphire interfacial region

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Abstract

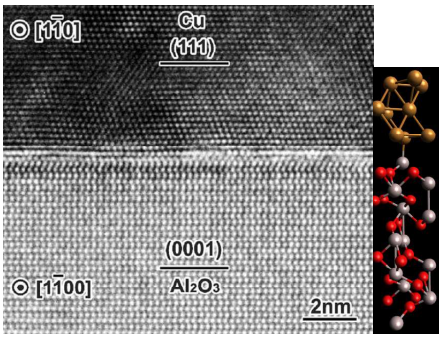
A method for reconstruction of atomistic models of dislocations and stacking faults in the interfacial region of heterostructures is presented. Its mathematical foundations come back to the algebra of the finite deformation fields related to introducing of discrete dislocations into an initially coherent interface. From the practical point of view the method concerns generation of interfacial regions with misfit/treading partial dislocations and stacking faults being formed in the interfacial region between crystal structures of different crystallographic type.

Keywords: atomistic models, dislocations, stacking faults, lattice distortion

1. Introduction

Recently, the possibility of experimental investigation of materials in the atomistic scale opened the need for computer modelling of the mechano-chemo-physical properties of a set of atoms forming the examined crystal structures. The real structures contain many crystallographic defects resulting from a non-perfect growth process as well as from a pure geometric reason resulting simply from the misfit of lattice spacings of crystal structures constituting a single heterostructure as a whole. In many heterostructures, the main crystallographic axes of the crystal grown differ from orientation of the main crystallographic axes of the substrate. It makes the atomistic reconstruction of such a heterostructure very complex, cf. GaN/Al_2O_3 [4] and Cu(111)/Al_2O_3(001).

2. Experimental evidence



$$\frac{9\,\mathrm{Cu}}{12\,\mathrm{Al}+18\,\mathrm{O}}$$

Misfit:
$7\% \approx \frac{1}{14}$

Figure 1: Sasaki et al., *Sci. Techn. Adv. Mater.* (2003).

The interface junctions of Cu/α-Al_2O_3 were investigated by many authors. A typical high resolution transmission electron microscope (HRTEM) image examined by Sasaki *et al.* [3] is shown in Fig. 1.

3. Perfect heterostructure assumed

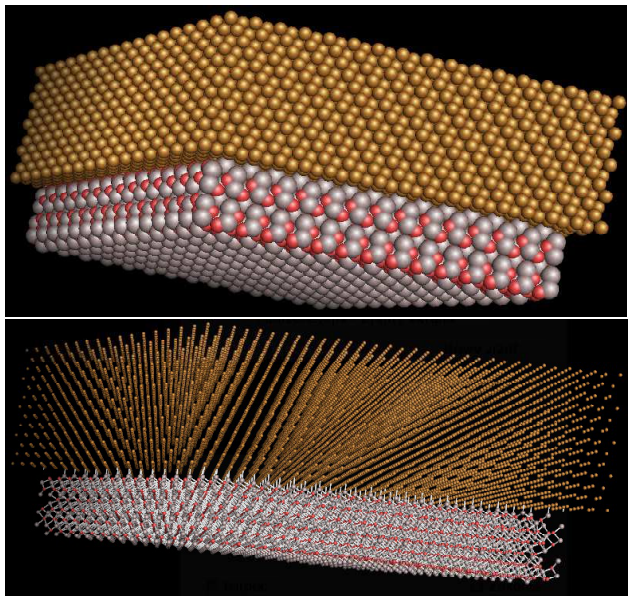


Figure 2: Template of periodic cell with copper crystal tensioned coherently to Al_2O_3.

* The research is developed in the framework of Project No 1566/B/T02/2010/38 founded by the Ministry for Science and Higher Education in Poland.

4. Dislocation network assumed

In the interfacial region we assume the net of partial dislocations and stacking faults shown in Fig. 3

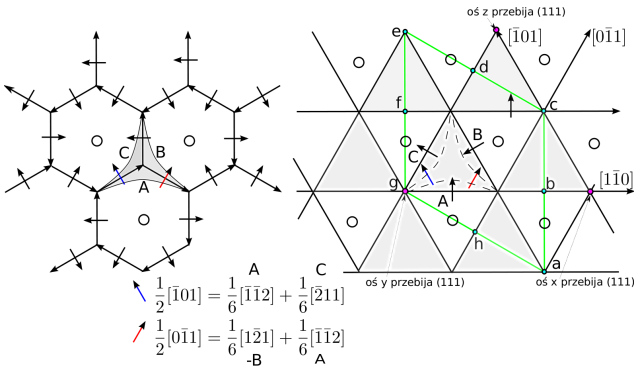


Figure 3: Dislocation network assumed. On the left, the complete dislocations dissociate to partial ones separated the SF triangles shown on the right hand, cf. Dimitriev et al. [2].

5. Visual Editor of Crystal Defects

In order to make easier the edition of dislocation structures it has been written a program [1]. The program, the Visual Editor of Crystal Defects (VECDs), has been written in C++, Qt4 and OpenGL. It is a wiswig editor which, by the use of computer mouse, makes possibility to rotate an next input the mixed dislocations and stacking faults into atomistic models of crystal structures.

6. After input of partial dislocations

Thanks to VECDs, a set of twelve partial dislocations and respective stacking fault triangles, shown schematically in Fig. 3, have been input sequentially into the initially coherent structure $Cu(111)/Al_2O_3$ shown in Fig. 2.

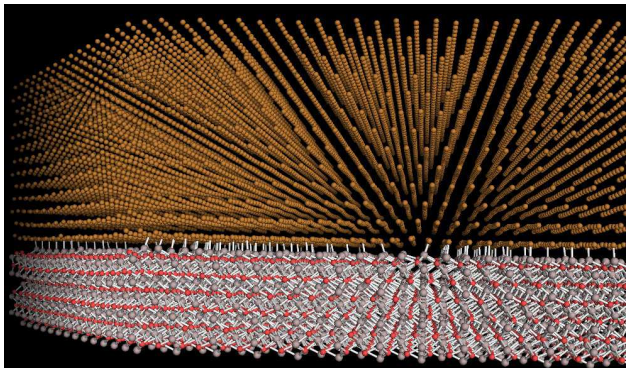


Figure 4: Relaxation by dislocations slips into periodicity cell

Such obtained atomistic model is undergone next relaxation by means the molecular dynamics (MD) and statics. The change of the potential energy is discussed.

7. Summary

The scheme presented above can be included to the methods of generation (preprocessing) the atomistic mesh forming the fixed set of defects in the crystal heterostructures. Contrary to the traditional MD methods, the present one is a deterministic method allowing to generate a fixed set of defects, e.g. the defects visible in HRTEM. The traditional methods are based on the input of initially perfect blocks of single crystals, which after MD relaxation tend to form an atomistic configuration of interface. Such obtained resultant configuration depends very strongly on the interatomic potential assumed. The method presented here allows to generate a fixed set of defects corresponding to the energetically stable or metastable configuration.

The resultant atomic positions obtained in the present approach can be used next as the input data for atomistic analysis with the use of molecular dynamics, statics, ab–initio, and other atomistic methods. The MD application is presented in our example.

8. Further plans

From the mathematical point of view the nonlinear method should be based on a non-commutative adding of finite distortion tensor fields corresponding to subsequently introduced dislocations. In the present approach a simpler method was applied being the linear form of the previous one. The present method is based on the traditional adding the distortion fields. The problem to solve consists in the proper reconstruction of atomistic displacements obtained by integration the lattice distortions. Such reconstructed atomistic displacement field is intersected by discontinuities corresponding to dislocation slip/climb planes being indispensable to introduce a set of misfit dislocation into the initially perfect atomistic model of heterostructure. Unfortunately, after introduction the first dislocation into a perfect coherent heterostructure the crystal planes are no longer flat. Therefore, the input of next dislocations should be done by means of the use of the curved slip/climb planes.

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