INTERACTION OF DEFECTS ON RECONSTRUCTED SILICON SURFACES

C.V. CIOBANU* AND V. TEWARY†

* Division of Engineering
Colorado School of Mines
Golden, Colorado 80401, USA
cciobanu@mines.edu

† Materials Reliability Division
National Institute of Standards and Technology
Boulder, Colorado 80305, USA

In the framework of elasticity theory, defects on crystal surfaces are modelled as multipoles placed on an elastic half-space and interacting via a power law determined by the type of multipoles considered [1]. Usually defects such as ad-atoms or vacancies have a strong dipole term, which determines an inverse-cube distance dependence ($1/d^3$) of their mutual interaction.

We have found that when the crystal surface is reconstructed (as are, for example, silicon surfaces), the reconstruction pattern itself drastically influences the interaction of defects placed on the reconstructed surface. In particular, in the case of Si(001)-2 $\times$ 1 surface, the interactions of dimer-vacancies become strongly anisotropic, concentrating mostly along the dimer row direction. Some evidence for this anisotropic dependence (which cannot be traced to the anisotropy of elastic constants of silicon) has been provided both by experiments [2,3] and theory [4,5]. Using embedded-atom and classical potentials, we calculate the interaction of several types of defects (ad-atoms, ad-dimers and dimer-vacancies) on the reconstructed Si(001) surface, and map it as a function of the mutual position of the defects on the surface. For all defect types and potential functions describing the atomic interactions, we found that the interactions of surface defects are affected by the reconstruction and do not follow the $1/d^3$ law predicted by the elastic theory of interacting dipoles on the surface. We construct a framework for describing the how the interaction of defects is "guided" by the reconstruction on the surface and also show that this guiding effect is rather general, and is not restricted to the (001) surface.

References

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