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Singular stress analysis near edge of a bump on substrate using molecular dynamics

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Advanced semiconductor products have structures with thickness and width in nanoscale. As the size of the structures reduces to a nanometer level, a ratio of their surface to volume increases. Generally, surface energy in deformable solids depends on surface strain. Surface stress and elasticity influence on the distribution of bulk stress near the surface. Interface stress and elasticity also exist in an interface of materials and characterize interface properties. In this study, singular stress at corners in an anisotropic two-dimensional joint structure under a tensile loading is analyzed using molecular dynamic (MD) method and the anisotropic elasticity theory using the boundary condition with interface stress and interface elasticity. Interface stress and interface elasticity are obtained through the MD analysis. Model for analysis is shown in Fig.1, where a bump of Au is built on a substrate of Cu. Stress distribution on the interface in the model that a tensile load of 100MPa is applied to the side surfaces of the substrate is calculated using MD method. In the present study, the model for analysis has a coherent interface. Furthermore, GEAM potential [1] is used. GEAM potential E is written as:

$$E_{tot} = \sum_{\alpha} \left\{ F_{\alpha}\left(\rho^{\alpha}\right) + \frac{1}{2} \sum_{\beta(\neq\alpha)} V_{\alpha\beta}\left(r^{\alpha\beta}\right) \right\} \tag{1}$$

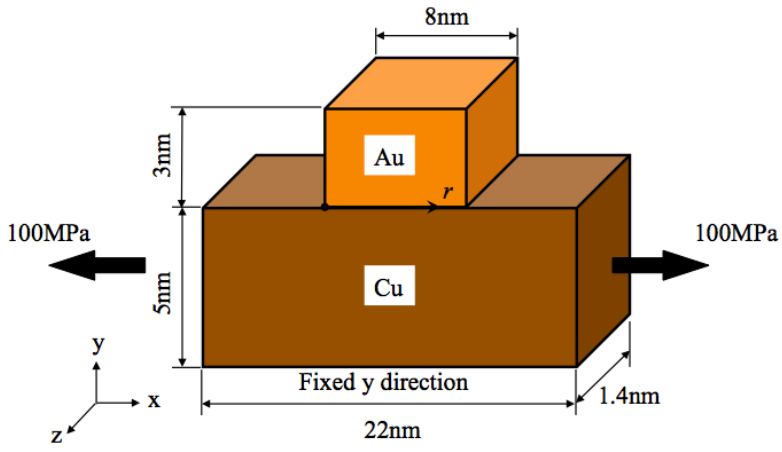

Fig.1 Model of analysis

where the embedding function F_{α} which gives a potential energy arising from embedding a particular atom in the electron density ρ^{α} at the site α, and $V_{\alpha\beta}$ is a pair interaction between atoms α and β whose separation is given by $r^{\alpha\beta}$.

The distribution of atomic stress near the corner of joint is calculated using the GEAM potential. Atomic stress for atom α is given by

$$\sigma_{ij}^{\alpha} = \frac{1}{\Omega^{\alpha}} \frac{\partial E_{\alpha}}{\partial \varepsilon_{ij}} \tag{2}$$

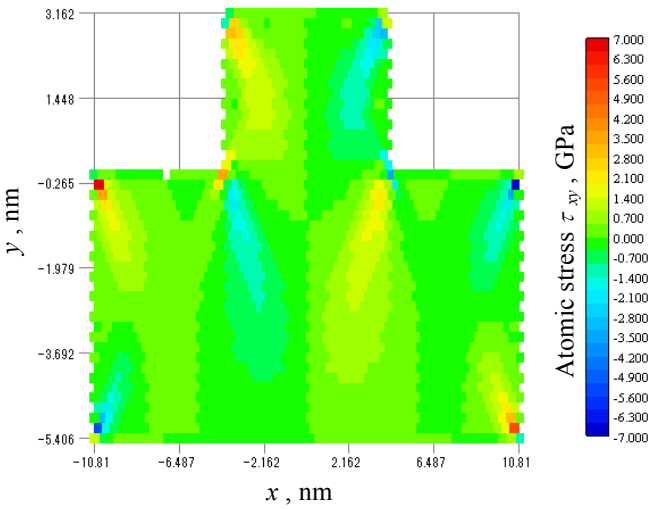

Fig.2 Stress distribution (τ_{xy})

where E_{α} is the total potential energy of atom α, Ω^{α} is the Voronoi volume of atom α and ε_{ij} is bulk strain.

Lattice constants in the model are modified so that the lattice constant in Au is agreed with that in Cu. The potential parameter r_e of Au is used in this model due to the modification of lattice constant. The distribution map of stress τ_{xy} in x-y plane is shown in Fig.2. It can be seen that a stress concentration of τ_{xy} occurs at the edge of the bump. Figure 3 represents the stress distribution along the interface against the distance from the bump corner. In Fig.3, a blue solid circle indicates the stress in Au side, a red solid circle represents the stress in Cu side, and a solid line represents a plot expressed by $K_{0xy} + K_{1xy} r^{-0.462}$, where coefficients are determined using a least square method. Here, $K_{0xy} = 0.85$ and $K_{1xy} = 1.45$. In the expression, the power index, 0.462, represents the order of stress singularity, which is obtained by solving the eigen equation derived from Stroh formalism. In the present study, the order of stress singularity considering interface stress and elasticity [2] will be calculated using Stroh formalism, and the validity of nanomechanics proposed by the authors will be discussed.

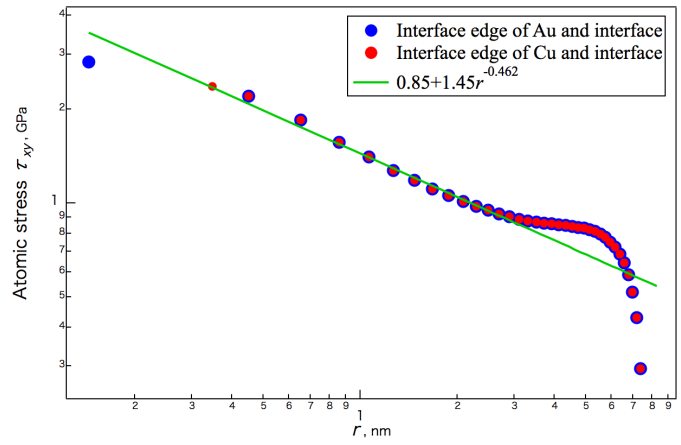

Fig.3 Distribution of stress τ_{xy} along the interface

In the present paper, the following conclusions are deduced.

(1) Stress distribution around a bump on the substrate under a tensile load was analyzed using MD.

(2) Stress distribution along the interface obtained by MD method was investigated using Stroh's formalism and eigen analysis.

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