Atomistic Calculation of Elementary Process of Adhesion during Forming

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ABSTRACT

The adhesion of a forming material on a tool strongly affects the friction behaviour especially in the small-scale forming. Hard coatings on the tool with less amount of adhesion during forming are required. Interfacial phenomena between tool and material during forming are difficult to be observed by experiments. Therefore, an atomistic-calculation analysis of the interaction between heterogeneous atoms, derived from first-principles electronic-state calculations, has been utilized for the study of an elementary process of adhesion during forming [1]. Before constructing the interactions [2] between NaCl-type ceramics coatings (TiN, VC and CrN) and Al, the calculated bulk and surface properties of these ceramics are verified by comparing with the reported experimental lattice parameter, bulk modulus and work function. The inter-atomic potentials for the constituent atoms in the transition metal carbide or nitrides at (100) and (110) surface planes and the Al atom, and the potentials between the first and the second layers of the Al atoms on the tool surfaces are constructed. Using these potentials, the molecular dynamics calculations for an ironing-type forming (the inclined tool moves over the material of which the bottom is fixed) are carried out. The comparison between the speed of a tool and an Al atom identifies whether the Al atom adheres on the tool. The change in number and distribution of the adhered atoms during ironing are compared between the three coatings.

The increase of the number of adhered atoms in the second layer onwards (the growth of adhesion) depends on the structure of the first layer of adhered Al atoms. If the location of the first nearest neighbour atom of Al first layer is equal to the second nearest neighbour atom of the tool surface, then the growth of adhesion occurred.

REFERENCES

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