Atomistic Calculation of Adhesion during Forming

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ABSTRACT

Hard coatings with smaller amount of adhesion during and after forming are required in this field. 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 adhesion during forming [1]. Before constructing the interaction [2] between 15 ceramic coatings (tool) and aluminum (material), calculated bulk and surface properties of the ceramics are verified by the reported experimental lattice parameter, bulk modulus and work function. Using the derived inter-atomic potentials for the interfaces between the constituent atom in transition metal carbides or nitrides and the Al atom, a molecular dynamics calculation with the geometry of ironing-type forming (the inclined tool moves over the material of which the bottom is fixed) is 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 with all the 15 combinations.

The number of adhered atoms in the first layer on the tools increases and saturates immediately. The behavior is common in all combinations. The change in number of adhered atoms in the second layer onwards shows wide variations.

The distribution of adhered atoms is analyzed by using a radial distribution function. 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 neighbor atom of Al first layer is equal to the second nearest neighbor atom of the tool surface, then growth of adhesion occurs.

REFERENCES

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