Adhesion between ferrite iron-iron/cementite countersurfaces: A molecular dynamics study

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Abstract:

The adhesive properties of Fe(110)/Fe(110) and Fe3C(001)/Fe(110) countersurfaces have been investigated by using classical molecular dynamics simulations. The simulation results show that Fe3C/Fe exhibits a relatively lower adhesion compared to the Fe/Fe. Additionally, the temperature dependence of the adhesive properties between 300–700 K has been examined. The results demonstrate that, with increasing the temperature, the values of the adhesion force and the work of adhesion continuously decrease in the case of Fe3C/Fe; they initially slightly increase up to 500 K then decrease in the case of Fe/Fe. Furthermore, the effect of lattice coherency between Fe/Fe has been examined and found to slightly reduce the adhesion. These results explain how carbides improve galling resistance of tool steel observed during dry sliding.

Keywords:

Molecular dynamics; Adhesion; Cementite; Iron; Commensurability

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