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Effect of Carbide Precipitates in Tool Steel on Material Transfer: A Molecular Dynamics Study

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Abstract : In sheet metal forming processes, accumulation and transfer of sheet material to tool surfaces, often referred to as galling, is the major cause of tool failure. Initiation of galling is assumed to occur due to local adhesive wear between two surfaces. Therefore, reducing adhesion between the tool and the work sheet has a great potential to improve the tool materials galling resistance. Experimental observations and theoretical studies show that the presence of primary micro-sized carbides and/or nitrides in alloyed steels may significantly improve galling resistance. Generally, decreased adhesion between the ceramic precipitates and the sheet material counter-surface are attributed as main reason to the latter observations. On the other hand, adhesion processes occur at an atomic scale and, hence, fundamental understanding of galling can be obtained via atomic scale simulations. In the present study, molecular dynamics simulations are used, with utilizing second nearest neighbor embedded atom method potential to investigate the influence of nano-sized cementite precipitates embedded in tool atoms. The main aim of the simulations is to gain new fundamental knowledge on galling initiation mechanisms. Two tool/work piece configurations, iron/iron and iron-cementite/iron, are studied under dry sliding conditions. We find that the average frictional force decreases whereas the normal force increases for the iron-cementite/iron system, in comparison to the iron/iron configuration. Moreover, the average friction coefficient between the tool/work-piece decreases by about 10 % for the iron-cementite/iron case. The increase of the normal force in the case of iron-cementite/iron system may be attributed to the high stiffness of cementite compared to bcc iron. In order to qualitatively explain the effect of cementite on adhesion, the adhesion force between self-mated iron/iron and cementite/iron surfaces has been determined and we found that iron/cementite surface exhibits lower adhesive force than that of iron-iron surface. The variation of adhesion force with temperature was investigated up to 600 K and we found that the adhesive force, generally, decreases with increasing temperature. Structural analyses show that plastic deformation is the main deformation mechanism of the work-piece, accompanied with dislocations generation.

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