Influence of Alloying Additives on The Adhesive Properties of Steels: Atomic Level Simulation

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Abstract

In the present work we report atomistic molecular dynamics simulation results on adhesion force between self-mated iron/iron, iron/vanadium, iron-cementite and iron/titanium surfaces has been determined and we found that iron/cementite surface exhibits lower adhesive force than that of iron/iron surface. The results showed that adhesion, quantified by the work of adhesion, decreased as the vanadium content increased and highest reduction was obtained for 10 at.% vanadium and 7.5 at.% for titanium. Furthermore, the variation of adhesion force with temperature was studied in the temperature range between 300-700 K and we found that the adhesive force generally is lowered at higher temperature.

Indexing terms/Keywords: molecular dynamics; galling; Vanadium; Titanium and adhesion.

Subject Classification: Physics- material science

Type (Method/Approach): Computational- atomistic simulation

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1. Introduction

In sheet metal forming operations, adhesion between surfaces is the one of the primary causes of wear where sheet material is transferred to the tool steel surface. Subsequent forming operations lead to scratching of the sheet surface by the transferred material that has gained in hardness due to severe plastic deformation and oxidation phenomena [1,2]. Several process parameters have been identified that influence the material transfer rate and both contact pressure and sliding speed lead to more severe forming conditions. Another parameter that depends on both pressure and speed is frictional heating of the surfaces during sliding. It has been observed that increasing temperature also increases the rate of adhesive wear [3]. Regarding materials, a significant difference is generally observed between different tool materials. For tool steels, the performance is increased as the volume fraction of primary precipitates, such as carbides, increases. This is often attributed to lower adhesion between the ceramic phase and the steel sheet work piece. Furthermore, it is reported that the type of precipitate seems to influence the tool life. For instance, tool steels with similar volume fraction, size and shape of precipitates were investigated in sliding against steel sheet. The results showed that a material containing(C,N) precipitates had substantially longer sliding distance until severe transfer of material occurred, as compared to a material with VC particles [4]. It was argued that the difference was due to differences in adhesion between V(C,N)/steel and VC/steel. However, using friction force microscopy to investigate friction and adhesion at the microstructural scale, little difference between different types of precipitates was found. Instead, largest difference was obtained for the steel matrix for different types of tool steel. Although the materials are based on a martensitic steel matrix, there will be some differences in chemical composition as type and content of alloying elements. The present work focuses on influence of M=V, Ti, and C in solid solution in steel on adhesion. Molecular dynamics simulations will be utilized to assess how different amounts of vanadium effects adhesion in a contact against an iron counter-surface.

2. Methodology

To study the adhesive properties, molecular dynamics simulations were carried out using modified embedded atom method (MEAM) potentials to describe the interaction between Fe-V [5] and Fe-C[6], Fe-Ti [7], respectively. The simulation cell consisted of two slabs where the lower slab was made of 15 layers of bcc iron oriented on [110] direction while the upper slab composed of iron and V or Ti alloying elements. In the case of carbon, we investigated the effect of carbon in form of cementite (Fe_3C) since this phase is commonly observed in low- alloying steels [8]. The dimension of the simulation box was 34.5×34.5×60 Å in –x, y and z direction, respectively. The atomic positions of the atoms located in the two bottom layers of the lower and the topmost two layers of the upper block were fixed. Before running the simulation, the two slabs were separated vertically by a distance greater than the cut-off radius of the interatomic potential. As a result, when the upper slab was pushed down towards the substrate, the initial force of adhesion between the two slabs was almost zero. Initially, the conjugate gradient (CG) method was utilized to minimize the simulation box, followed by thermal equilibration to 300 K for 200 ps using a Nosé-Hoover thermostat.

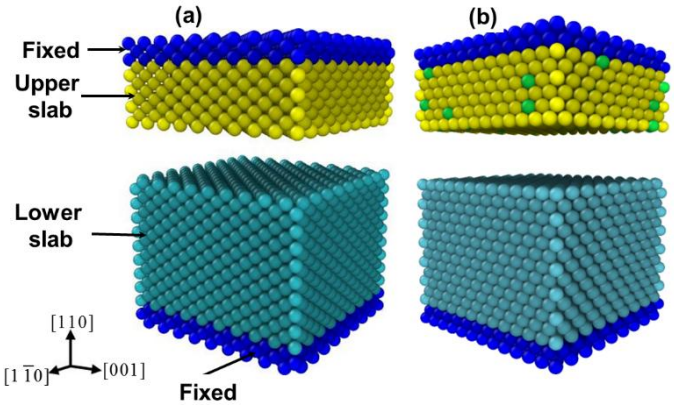

Fig. 1. Schematic illustration showing MD model used to study adhesion between two surfaces. (a) Fe/Fe and (b) Fe/Fe-M.

During loading stage, the upper slab was pushed downward to the lower slab by applying a constant velocity of 20 ms^{-1} to the fixed atoms, while a velocity of -20 ms^{-1} was kept during the unloading stage. All MD simulations were performed using open-source software LAMMPS[9] and the free software tool OVITO is used for visualizing the local atomic structure [10].

3. Results and Discussion

Figs. 2 Shows typical force-separation curves for Fe/Fe, Fe/Fe_3C, Fe/Fe-V and Fe/Fe-Ti countersurfaces. The adhesive forces were determined by summing all normal force exerted from upper slab on the lower slab atoms. The adhesive forces are 237, 135.8 228.5 and 195 nN for Fe/Fe, Fe/Fe-V, Fe/Fe_3C and Fe/Fe-Ti, respectively. It is noticed that while the value of adhesive force on the case of Fe/Fe and Fe/Fe_3C counterfaces is comparable, it is significantly reduced by about 18% and 43% in the case of Fe/Fe-Ti and Fe/Fe-V counterfaces, respectively. Our simulation results are consistent with the results of DFT studies where it is reported that when reduction of adhesive force when adding carbide or vanadium [11]. Furthermore, experiments have shown that an improved wear resistance was observed for tool steels containing vanadium and carbides [12–15].

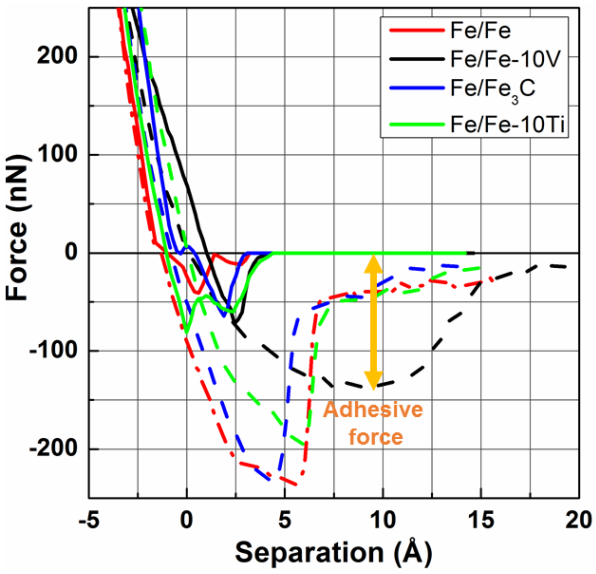

Fig. 2. Typical force-separation curves of Fe/Fe,V/Fe and Fe_3C/Fe counter surfaces at T=300 K. Solid lines represent approaching stage, while dashed line mark retraction stage.

In addition to the adhesive forces, the work of adhesion W_{ad} [16] was used as an indicator of adhesion. W_{ad} is defined as the energy required to separate two surfaces from the equilibrium position to infinity [10]. The value of W_{ad} was calculated from the following equation

$$W_{ad}=\gamma_A+\gamma_B-\gamma_{AB} \quad (1)$$

Here γ_A, γ_A and γ_{AB} represent surface energy of slab A, slab B and interfacial energy of AB, respectively. Their values can be calculated as follows

$$\gamma_A \approx \frac{E_A}{\text{Area}}$$

$$\gamma_B \approx \frac{E_B}{\text{Area}}$$

$$\gamma_{AB} \approx \frac{E_A + E_B - E_{AB}}{\text{Area}}$$

where E_A and E_B correspond to the energy differences between the bulk system and a system with a free surface, respectively. The value of E_{AB} can be determined by integrating the attractive portion of the force-displacement curve during retraction stage then subsequently divided by the lateral area of the computational cell [17].

In order to examine the effect of alloying additives on adhesion properties, we studied the compositional dependence of adhesive properties for Fe/Fe-xM where (M=V and Ti) and (x=2.5, 5, 7.5, 10, 12.5, 15 and 17.5 at.%), at 300 K. Fig. 3 displays the variation of W_{ad}, calculated by Eq.(1), with alloying additive contents. Generally, the value of W_{ad} initially decreases until reaching a minimum then increases again with alloying composition. While both curves exhibit a minimum, it is noticed that the lowest value of W_{ad} occurs at 10 at. % for vanadium whereas the lowest W_{ad} for Ti obtained at 7.5 at.%.

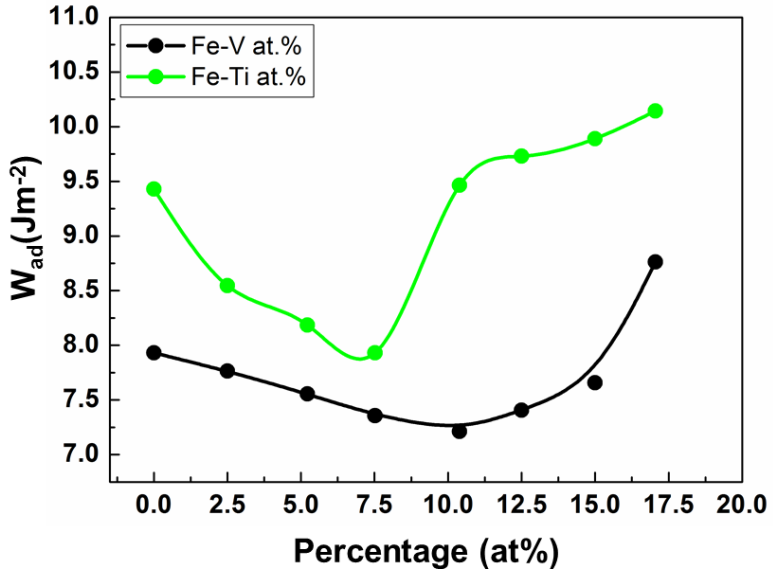

Fig. 3. Variation of adhesive force with alloying additives at 300 K.

Another important factor that affect the adhesive properties between two surfaces is the temperature. Hence, the temperature dependence of wad was examined in the temperature range between 300-700 K for Fe/Fe, Fe-Fe-10V, Fe/Fe-10Ti and Fe/Fe_3C. In the case of Fe/Fe, it is found that the value of Wad initially increases up to 500 K then decreases for higher temperature. Similar behavior was reported by Atomic Force Microscopy (AFM) experimental studies on nanoscratching of ferritic iron by diamond tip[18]. In contrast, the adhesive forces were found to continuously decrease with increasing temperature for Fe/Fe_3C, Fe/Fe-10V and Fe/Fe-10Ti counter surfaces. This finding is consistent with density functional theory (DFT) results displaying a reduction of adhesive properties between metal/carbides surfaces[19,20]

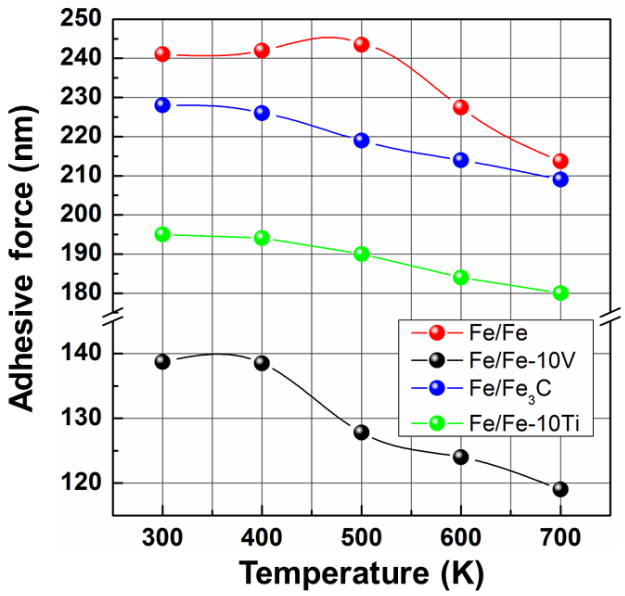

Fig.4. Influence of temperature on the adhesive force for different ferritic alloys.

As has been reported in [21,22] during nanomachining, the tool/sheet interface temperature increases and subsequently leads to changing the adhesive force. Therefore, we have investigated the variation of adhesive force in the temperature range from 300K to 700K. Fig. 4. Displays the variation of adhesive force with temperature for Fe/Fe, Fe-10V, Fe/Fe_3C and Fe/Fe-10Ti counterfaces. For Fe/Fe counter surfaces, we found that the adhesive force slightly increases upto 500K and then decreases with increasing temperatures. Similar behavior was experimentally observed during nanoscratching of iron by diamond tip[18]. On the other hand, increasing the temperature in the case of Fe/Fe_3C leads to decreasing adhesive force.

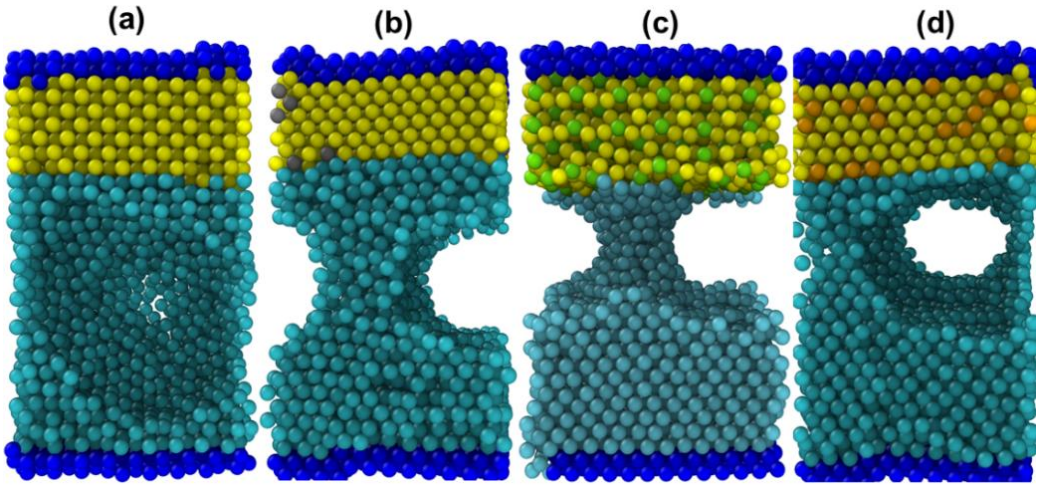

Fig. 5. MD Snapshots showing the material transfer observed by the end of retraction process for (a) Fe/Fe, (b) Fe/Fe-10V, (c)Fe/Fe_3C and Fe/Fe-10Ti.

Fig. 5 dsiplays MD snapshots for the various counter-surfaces. It is evident from Fig. 5 that the amount of material transfer from the bottom surfaces varies with alloying elements of of the upper surfaces. The above results imply that alloying of steel can be an additional way of reducing adhesion and adhesive wear and depending on the work material, the tool chemical composition may be tailor made for low adhesion.

4. Conclusions

The present work included molecular dynamics simulations of adhesive properties of iron alloyed with vanadium in contact against an iron countersurface. The results showed that the work of adhesion decreased as vanadium or Titanium content increased up till 10 or 7.5 at.%. At this value a decrease of approximately 10 % was observed. Higher vanadium or titanium content led to an increase in adhesion again. The results were discussed in terms of alloying being a method of decreasing adhesion in sliding contacts suffering from adhesive wear. Increasing temperature above 500 K leads to a decrease of adhesive force for all samples considered in this work.

Conflicts of Interest

The author declares that there is no conflict of interest.

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