Mechanisms of Graphite Lubrication

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Friction and wear in graphite show a strong dependence on moisture, the causes of which are not yet understood. By means of quantum chemical methods the influence of water on friction and wear processes is simulated on an atomic scale. Changes in the atomic structure provide new approaches to explain the frictional properties of graphite.

Keywords: tribology, graphite, lubrication mechanisms, atomistic simulation

1. Introduction

Graphite is one of the oldest technically used dry lubricants. A popular explanation for its lubrication properties is based on the lamellar structure of graphite. Since the layers interact with each other only by weak van-der-Waals forces, it is assumed that they can move against each other like in a deck of playing cards. This model offers a simple explanation for the lubricating properties of graphite [1]. However, it has been known since the 1930s that graphite loses these properties in dry environments [2]. Subsequently, there were various approaches to explain this, such as the saturation of dangling bonds on graphite planes or the increase of the interlayer distance due to water intercalation. However, these did not provide a satisfactory explanation for the lubricating properties of graphite [3] and the underlying mechanisms are still not understood today.

2. Methods

In this work we used tight-binding molecular dynamics simulations to investigate the influence of water on the lubricating properties of graphite. The small model systems that we used are shown in Figure 1. In an extensive parameter study we investigated the influence of pressure and water quantity in the gap.

3. Discussion

It turned out that the lubricating properties are essentially determined by 3 effects: If there is a large amount of water in the gap, the surfaces are completely separated by a thin film of water (Fig. 1a) which leads to low friction in the system. A small amount of water in the gap can either lead to cold welding of the surfaces with correspondingly high friction (Fig. 1c), or an aromatic structure can form at the interface after a certain time (Fig. 1b). This in turn leads to a separation of the surfaces from each other and thus to low friction (Fig. 1d). Overall, our results provide a promising new approach to explain the humidity dependence of the frictional properties of graphite.

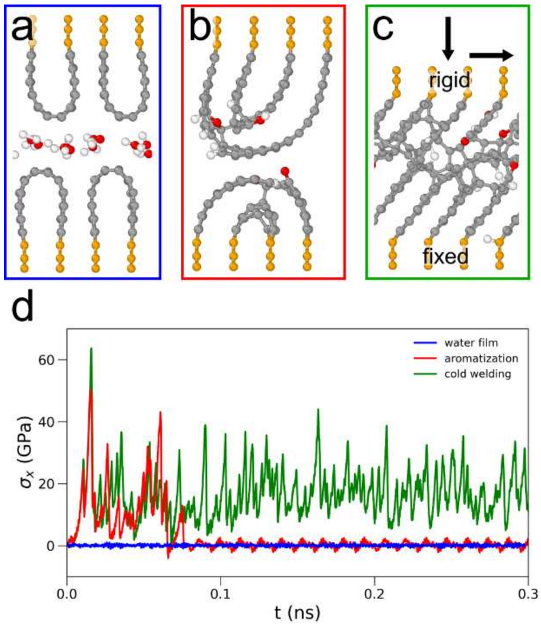

Figure 1: Examples for the influence of water on friction and wear in graphite-graphite contacts. A large amount of water between the surfaces leads to separation by a thin film of water (a). Small amounts of water can cause aromatic structures to form at the interface (b), or the surfaces to cold weld and amorphize while shearing (c). Aromatization and a water film between the surfaces result in low shear stresses during sliding (d).

4. References

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