Interlayer friction behavior of molybdenum ditelluride by AFM nano-manipulation

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The interlayer friction behavior of two-dimensional transition metal dichalcogenides as crucial solid lubricants has attracted extensive attention in the field of tribology. In this study, the interlayer friction is measured by laterally pushing the $MoTe_2$ powder on the $MoTe_2$ substrate with the atomic force microscopy (AFM) tip, and density functional theory simulations are used to rationalize the experimental results. The results indicate that the friction coefficient of the 1T'-$MoTe_2$ /1T'-$MoTe_2$ interface is 2.025 × 10^{-4}, which is lower than that of the 2H-$MoTe_2$ /2H-$MoTe_2$ interface (3.086 × 10^{-4}), while the friction coefficient of the 1T'-$MoTe_2$ /2H-$MoTe_2$ interface is the lowest at 6.875 × 10^{-5}. The lower interfacial friction of 1T'-$MoTe_2$/1T'-$MoTe_2$ compared to 2H-$MoTe_2$ /2H-$MoTe_2$ interface can be explained by the relative magnitudes of the ideal average shear strengths and maximum shear strengths obtained based on the interlayer potential energy, while the smallest interlayer friction of the 1T'-$MoTe_2$ /2H-$MoTe_2$ heterojunction is related to the weak interlayer electrostatic interaction and the weakening of the potential energy corrugation caused by the incommensurate contact. This work suggests $MoTe_2$ has comparable interlayer friction properties to MoS_2 and is expected to reduce interlayer friction in the future by inducing the 2H-1T' phase transition.

Introduction

Two-dimensional materials have drawn incredible research interest in recent years owing to their unique structure and excellent physical and chemical properties. Among various two-dimensional materials, transition metal dichalcogenides (TMDCs), represented by MoS_2/ $MoTe_2$, have become popular materials in the field of tribology because of their excellent tribological properties under extreme conditions such as space environment. Due to weak interlayer incteraction and strong intralayer bonding, TMDCs are prone to interlayer sliding and their interlayer friction behaviors have been extensively studied from experimental and theoretical simulations. Here, the interlayer friction and friction coefficient were determined by laterally pushing the $MoTe_2$ powder to slide on the $MoTe_2$ substrate using the AFM tip.

Experiment and results

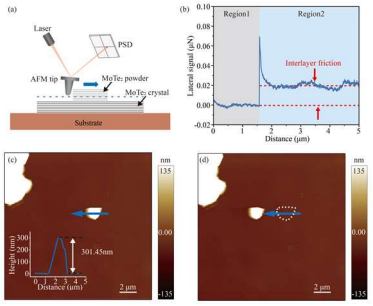

Fig 1. Interlayer friction force of $MoTe_2$

The interlayer friction force of MoTe2 is measured in Fig1(a). The friction curve shown in Fig. 1(b) corresponds to pushing the 1T'-$MoTe_2$ powder on the 2H-$MoTe_2$ crystal substrate from the position shown in Fig. 1(c) to the position shown in Fig. 1(d) along the blue arrow.

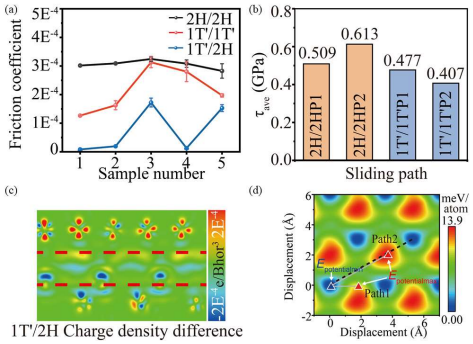

Fig 2. Results and density functional theory (DFT) simulations

In Fig 2(a), the experimental difference in the average interfacial friction coefficient between 1T'/1T' (2.025 × 10^{-4}) and 2H/2H (3.086 × 10^{-4}) can be explained by the relative magnitude of the interlayer shear strength in Fig 2(b), which was calculated through DFT simulations. Additionally, the low friction coefficient of 6.875 × 10^{-5} observed at the 1T'/2H interface is attributed to the weak interlayer Coulomb interaction and the potential energy corrugation modulation caused by the lattice mismatch between the layers in Fig 2(c). Fig. 5(d) shows different sliding paths in Fig 2(b).

In summary, a straightforward and effective method was employed to measure interlayer friction, where the 1T'/1T' bilayer $MoTe_2$ structure has lower interlayer friction than the 2H/2H structure and the 1T'/2H heterogeneous interface is most susceptible to interlayer sliding.