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Atomistic Analysis of 4H-SiC/Titanium Nanoscale Friction Behavior under the Effects of Normal Load and Temperature Using Molecular Dynamics

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Abstract

In this study, the frictional behavior of the contact between silicon carbide and titanium is investigated using molecular dynamics simulation. To model the system, rectangular blocks of 4H-SiC and titanium are constructed, and the interatomic interactions are described using the Tersoff, embedded atom method (EAM), and Lennard–Jones potentials. The simulation procedure involves the application of a normal load followed by the sliding motion of the titanium block over the SiC surface, and the coefficient of friction is calculated as the ratio of the averaged friction force to the applied normal force. The effects of normal load and temperature on the coefficient of friction are systematically analyzed. The results indicate that increasing the applied normal load leads to a reduction in the coefficient of friction, while variations in temperature result in a linear yet stable frictional behavior throughout the simulation. This study provides atomistic insight into the SiC–Ti contact and contributes to a deeper understanding of the mechanisms governing friction at the nanoscale, with potential implications for the design and optimization of advanced tribological systems.

Keywords: Silicon carbide; Titanium; Molecular dynamics; Coefficient of friction; Nanotribology.

1. Introduction

Tribological phenomena at heterogeneous material interfaces are crucial for the performance and durability of engineering components, particularly as industries seek lightweight and high-strength materials. Advanced ceramics like silicon carbide (SiC) and metallic alloys such as titanium are increasingly utilized in sectors like aerospace and biomedical engineering due to their remarkable properties—SiC offers hardness and wear resistance, while titanium is known for corrosion resistance and strength. Despite their individual advantages, the tribological behavior of SiC and titanium when they interact as a ceramic-metal contact pair is not well understood at the nanoscale, where atomic interactions influence friction and wear. Traditional experimental methods fail to capture atomic-scale phenomena, making molecular dynamics (MD) simulations vital for investigating these mechanisms. Most prior MD studies have concentrated on either SiC self-contact or titanium-based materials, but research on the direct sliding contact between 4H-SiC and titanium under varying conditions is limited. There is a need to explore the impact of external loading and thermal conditions on the frictional response of the SiC-Ti interface to enhance the performance of ceramic-metal tribological systems.

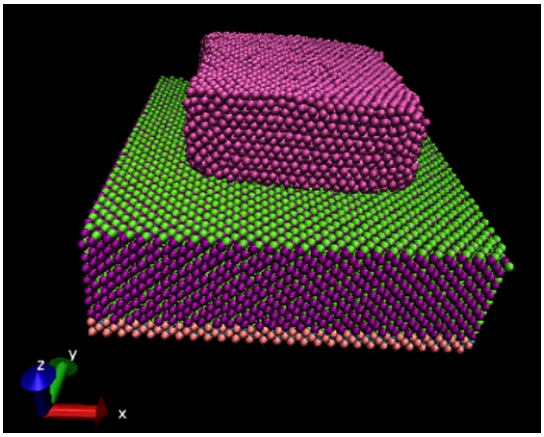

Figure 1. illustrates the atomistic model used for molecular dynamics simulations

2. Simulation Mthodlogy

The atomistic model consisted of two rectangular crystalline blocks representing the 4H-SiC substrate and the titanium counterface. The SiC crystal structure was initially generated using Atomsk and subsequently imported into the LAMMPS simulation package for molecular dynamics calculations. A titanium block with smaller dimensions was positioned above the SiC substrate while maintaining an initial separation distance to eliminate undesired atomic overlap before loading. The interatomic

interactions within the silicon carbide substrate were described by the well-established Tersoff potential, which accurately reproduces the covalent bonding characteristics of SiC. The titanium atoms were modeled using the Embedded Atom Method (EAM) potential because of its capability to capture many-body metallic interactions. Cross-interface interactions between silicon carbide and titanium were represented by the Lennard–Jones potential, whose parameters were determined from mixing rules based on the individual atomic parameters of titanium, silicon, and carbon. Initially, a prescribed normal load was gradually applied to the titanium block using the addforce command until stable contact was established between the two materials. Subsequently, the titanium slider moved across the SiC surface with a constant sliding velocity using the move command. During the entire simulation, tangential and normal interaction forces were continuously recorded. The friction coefficient was calculated from the ratio of the averaged tangential force to the corresponding normal load after steady-state sliding conditions had been achieved. To investigate the influence of operating conditions, two independent parametric studies were performed. The first series evaluated the effect of four different normal loads while maintaining a constant temperature of 300 K. The second series investigated temperature-dependent friction under a constant normal load over a wide temperature range. These simulation conditions enabled a systematic evaluation of the atomistic friction behavior at the heterogeneous SiC–Ti interface.

3. Result and Discussion

The obtained results clearly demonstrate that the frictional response of the SiC–Ti interface strongly depends on the applied normal load. Increasing the normal load consistently reduced the calculated friction coefficient throughout the simulations. This trend can be attributed to the gradual reduction in the relative contribution of adhesive interfacial forces as externally applied mechanical loading becomes dominant. Under higher normal loads, the contact behavior gradually transitions from adhesion-controlled friction toward load-controlled friction, resulting in a lower friction coefficient despite the increased contact force. The influence of temperature exhibited a considerably different behavior. Although slight fluctuations in friction coefficient were observed throughout the investigated temperature range, no significant monotonic increase or decrease was detected. The relatively stable frictional response indicates that the thermal energy introduced within the selected temperature interval was insufficient to substantially modify the dominant deformation and sliding mechanisms occurring at the interface. Consequently, the atomic configuration of the contact region remained relatively stable during sliding. The atomistic observations further indicate that friction generation within the heterogeneous interface is primarily governed by interfacial atomic interactions rather than macroscopic friction laws. These findings are consistent with previous molecular dynamics investigations reporting that nanoscale friction frequently deviates from classical Amontons behavior because adhesive interactions, local atomic rearrangements, and interface stability become increasingly dominant. The reliability of the adopted simulation methodology was further confirmed through validation against previously published tribological data for dry SiC–SiC contact. The predicted friction coefficient exhibited satisfactory agreement with the reference results, demonstrating that the selected interatomic potentials accurately reproduce the tribological behavior of silicon carbide-based systems and can therefore be confidently employed for analyzing heterogeneous SiC–Ti interfaces.

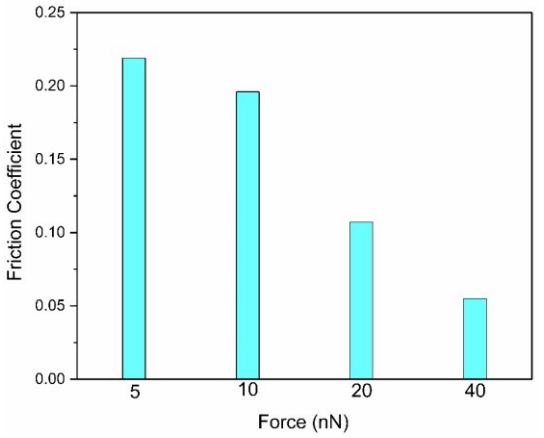

Figure 2. the friction coefficient decreases with increasing normal load, indicating a gradual transition from adhesion-dominated to load-controlled friction.

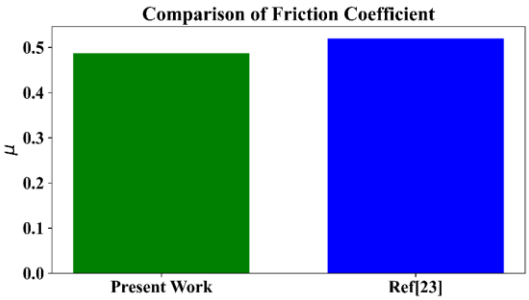

Figure 3. compares the predicted friction coefficient with previously published data, confirming the reliability of the adopted molecular dynamics model.

4. Conclusion

This study employed molecular dynamics simulation to investigate the atomistic friction behavior of a heterogeneous 4H-SiC/titanium sliding interface under different normal loading and thermal

conditions. The adopted computational framework successfully captured the evolution of interfacial forces and provided detailed insight into the friction mechanisms governing ceramic–metal contact at the nanoscale. The simulation methodology, incorporating the Tersoff, Embedded Atom Method (EAM), and Lennard–Jones interatomic potentials, proved capable of accurately describing the interactions within and between the constituent materials. Validation of the simulation model against previously published SiC–SiC friction data further confirmed the reliability of the adopted atomistic approach. The obtained results revealed that the coefficient of friction is strongly dependent on the applied normal load. An increase in normal load resulted in a noticeable reduction in the friction coefficient, indicating a transition from adhesion-dominated friction toward load-controlled interfacial behavior. In contrast, temperature exhibited only a limited influence on the friction coefficient within the investigated range. Although minor nonlinear fluctuations were observed, the overall frictional response remained relatively stable, suggesting that the applied thermal energy was insufficient to induce significant changes in the dominant atomistic deformation and sliding mechanisms. The present findings demonstrate that friction at the 4H-SiC/Ti interface is primarily governed by atomic-scale interactions rather than by classical macroscopic friction theories. Consequently, molecular dynamics simulation provides an effective tool for understanding tribological phenomena that cannot be directly observed through conventional experimental techniques. The atomistic interpretation presented in this work contributes to a more comprehensive understanding of heterogeneous ceramic–metal interfaces and provides valuable guidance for the development of advanced tribological materials From an engineering perspective, the outcomes of this research may support the optimization of material selection and interface design in applications where silicon carbide and titanium operate under severe contact conditions, such as aerospace structures, biomedical devices, precision manufacturing systems, and micro/nano-electromechanical components. Furthermore, the developed simulation methodology can be extended to investigate the influence of additional parameters, including sliding velocity, crystallographic orientation, surface roughness, lubrication conditions, and different ceramic–metal combinations, thereby providing a foundation for future nanoscale tribological investigations.

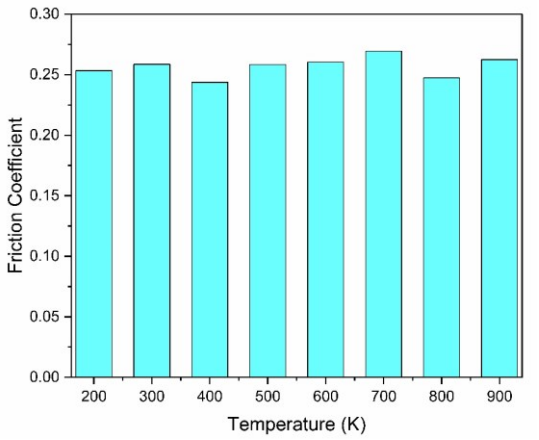

Figure 4.demonstrates that the friction coefficient remains relatively stable over the investigated temperature range despite minor nonlinear fluctuations.

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