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Tribological Properties of Selected Vanadium Oxide Stoichiometries Studied with Reactive Molecular Dynamics

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Providing effective lubrication at high temperatures/pressures and in oxidative environments is relevant for various industrial applications, such as turbomachinery and cutting tools [1,2]. Promising solutions for such conditions are oxidation-resistant hard coatings consisting of binary or ternary films (Cr-N, Ti-N, Cr-Al-N, Ti-Al-N) doped with an additional element which can diffuse to the surface of the coating and form an oxide layer that serves as a lubricant. Vanadium became a popular dopant since its oxides melt at considerably low temperatures, hence providing liquid lubrication.

The amount of oxygen present in an oxidative environment can be taken as a study parameter, leading to the consideration of different vanadium oxide stoichiometries. This study aims to explore the tribological performance of under-oxidized vanadium lubricants, selected in accordance with available experimental studies [3].

We present a reactive molecular dynamics study on the tribological properties of five vanadium oxide stoichiometries {V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2} at elevated temperatures {600, 800, 1000} [K] and pressures {1, 2, 3, 4} [GPa]. Our tribological system consists of two rigid V_2O_5 layers, modeling two solid surfaces in a tribocontact, and a vanadium oxide with stoichiometry labeled as V_xO_y, confined between them. Under the imposed working conditions, all studied vanadium oxides were amorphous.

We have employed an atomistic model within the *ReaxFF* (reactive force field) potential to describe the interactions of vanadium and oxygen atoms. Sliding simulations were implemented in the *reax/c* package of the *LAMMPS* code [4].

By applying a linear fit on the dependence of the sliding force F_x on the normal load F_z:

$\mathrm{F}_x = COF \cdot F_z + F_x^0$,

we extracted the coefficient of friction COF and the sliding force at zero load F_x^0 (adhesion component of the friction force). At a fixed temperature, we did not notice significant changes of the friction coefficient with stoichiometry. The values which we obtained for the COF (~0.2 at 600 K, ~0.15 at 800 K and ~0.1 at 1000 K) are in good agreement with the previously determined results for amorphous V_2O_5 lubricant at the same temperatures [5]. We concluded that all considered V_xO_y stoichiometries (i.e., under-oxidized vanadium) are going to be an effective lubricant. The friction coefficient COF decreases with the increase of the temperature. We observed the increasing trend of the adhesion-related offset of the friction force F_x^0 with the decrease of the oxygen content in V_xO_y lubricants and explained it by the more-pronounced tendency of vanadium atoms from V_xO_y to bond with oxygen atoms from V_2O_5 in oxygen-poorer environments.

Our study on vanadium oxide lubricants provides a reference which is relevant for the design of vanadium doped oxidation-resistant hard coatings.

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