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Reactive Molecular Dynamics Study on the Tribological Properties of Selected Vanadium Oxides

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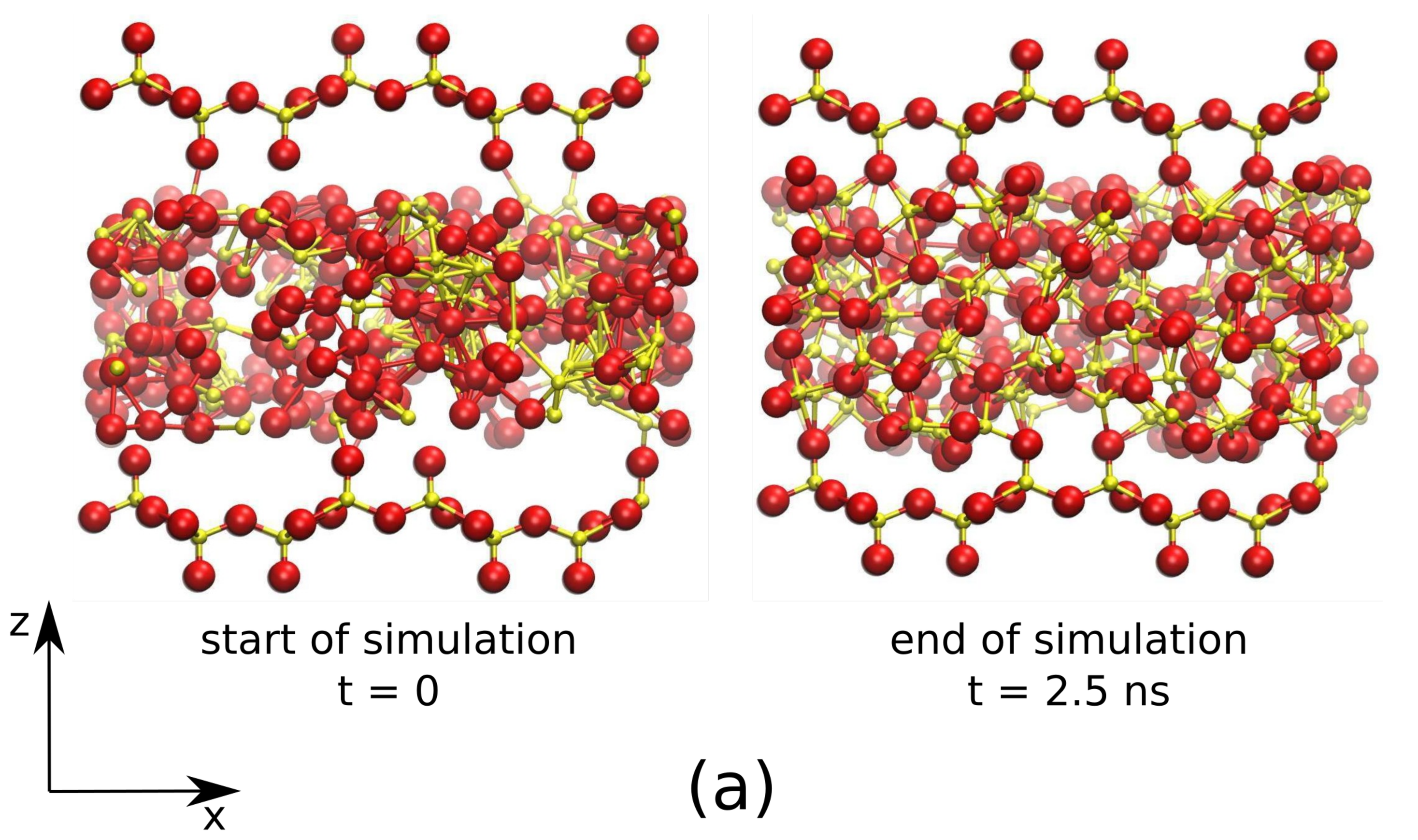
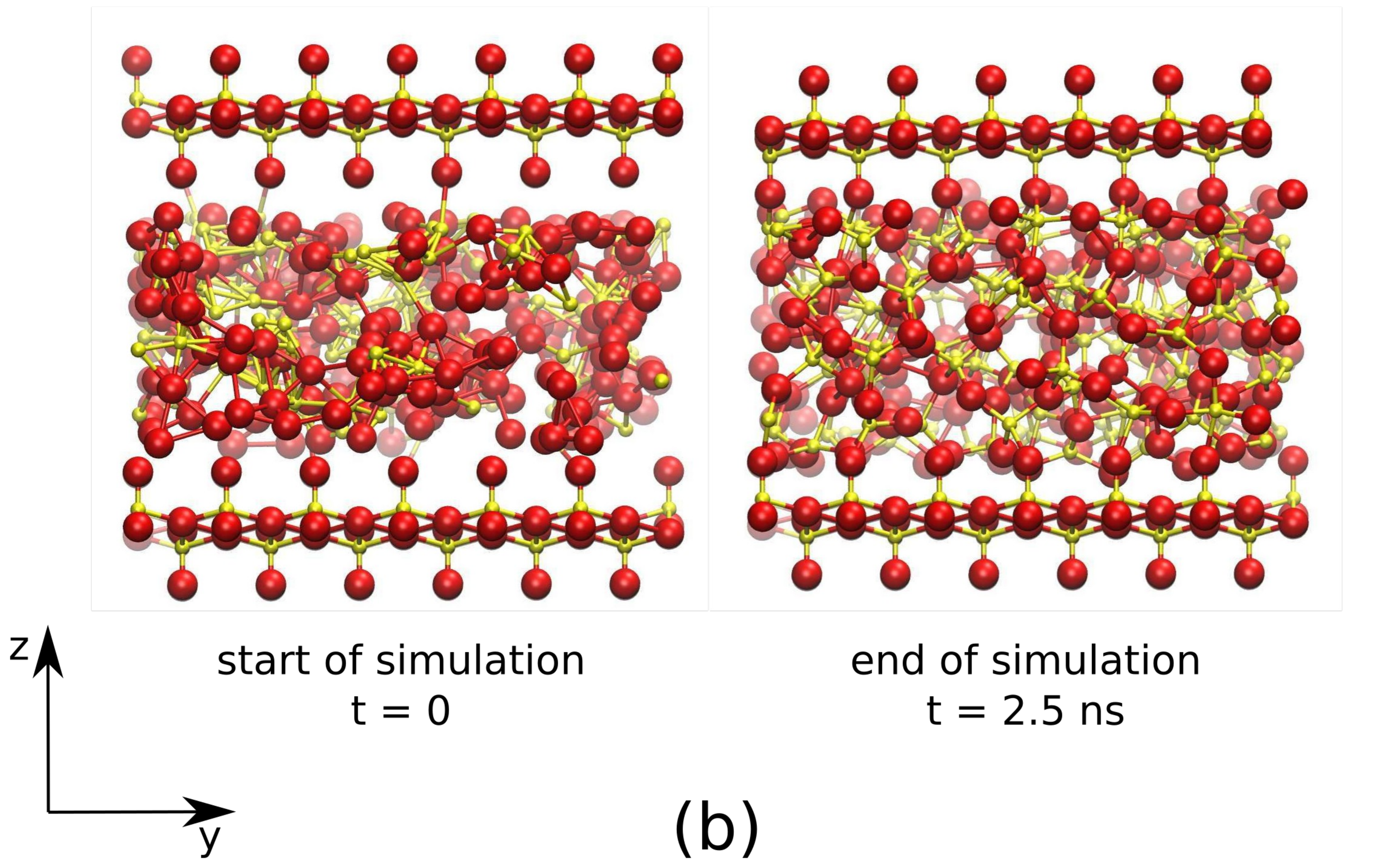
Introduction

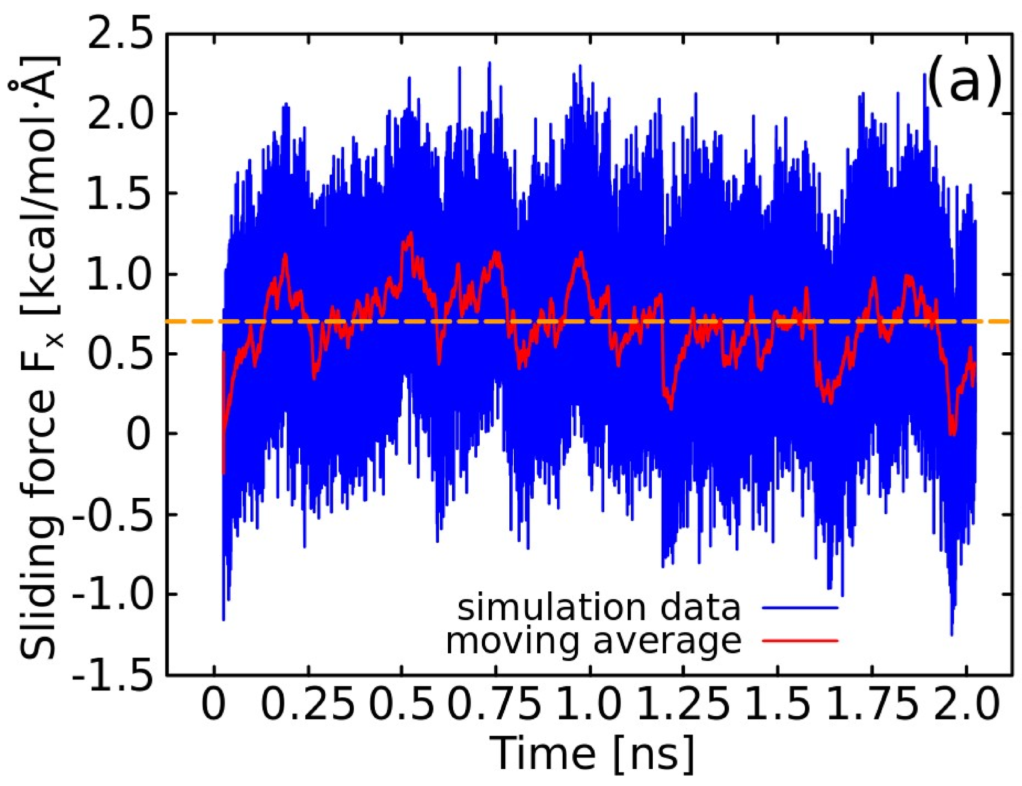
- Friction accounts for the losses of approximately one quarter of the global energy production. Providing effective lubrication at high temperatures and pressures and under oxidation is relevant for turbomachinery, machining tools, aerospace industry.
- Hard and oxidation-resistant coatings consist of binary or ternary films (Cr-N, Ti-N, Cr-Al-N, Ti-Al-N) doped with an additional element. Vanadium gained popularity since its oxides reduce friction and they melt at relatively low temperatures, hence providing liquid lubrication.
- Vanadium diffuses to the surface of the coating, reacts with oxygen and forms an oxide of a certain stoichiometry (VxOy) which serves as a lubricant. The motivation of our research: how does the stoichiometry impact the tribological properties of VxOy lubricants, under the aforementioned conditions.

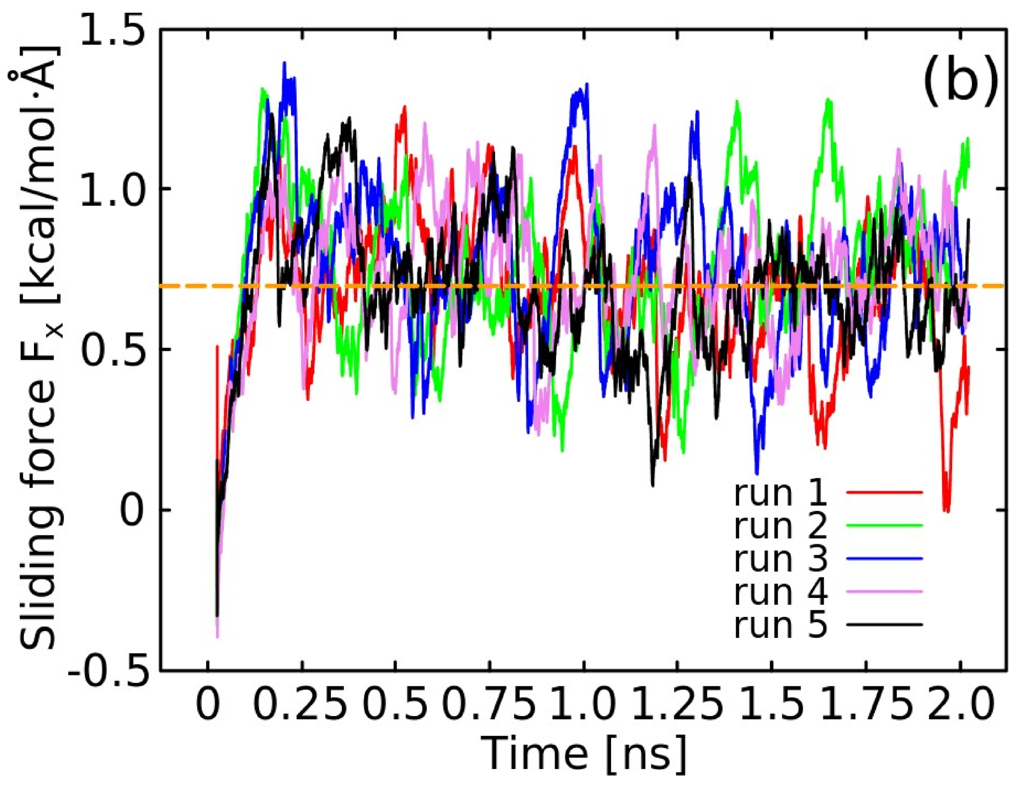
Simulation setup



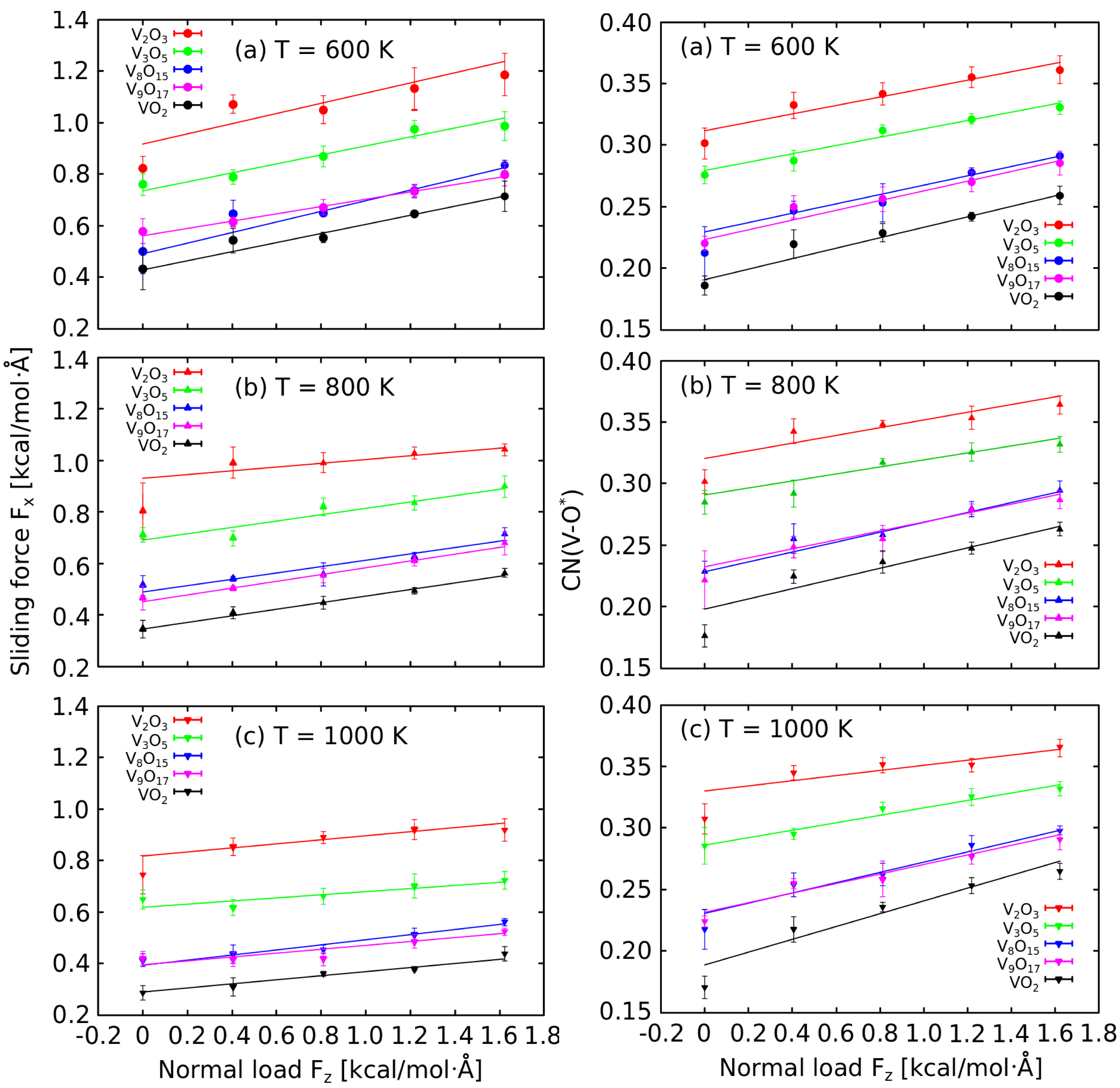


Sliding simulations

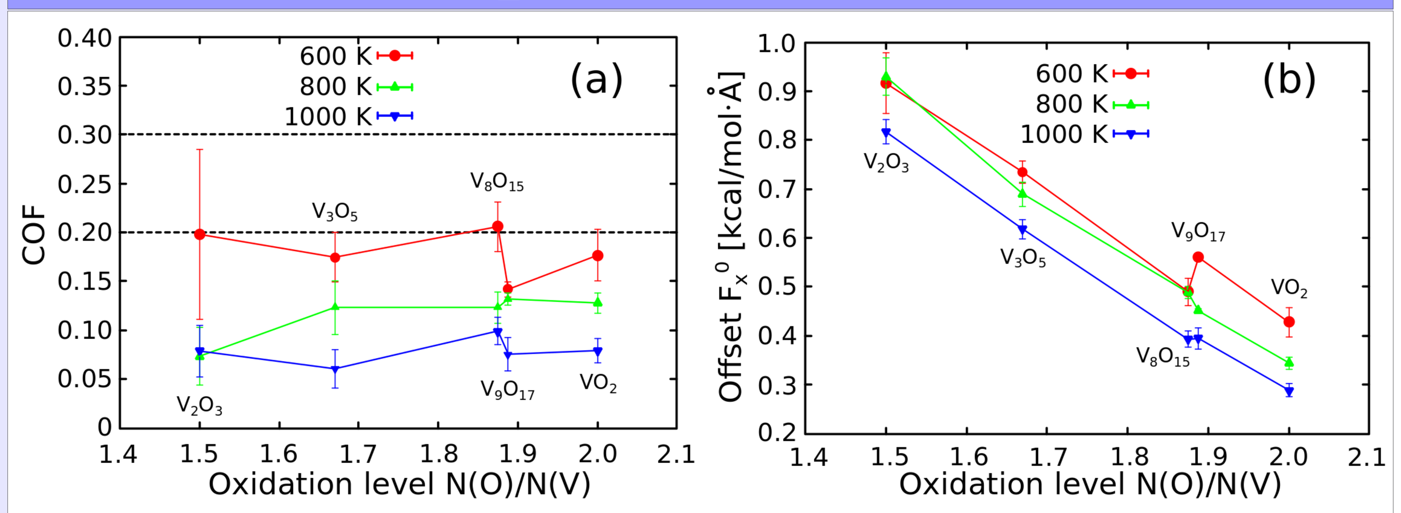




Sliding force Fx and CN(V-O*) vs. normal load Fz

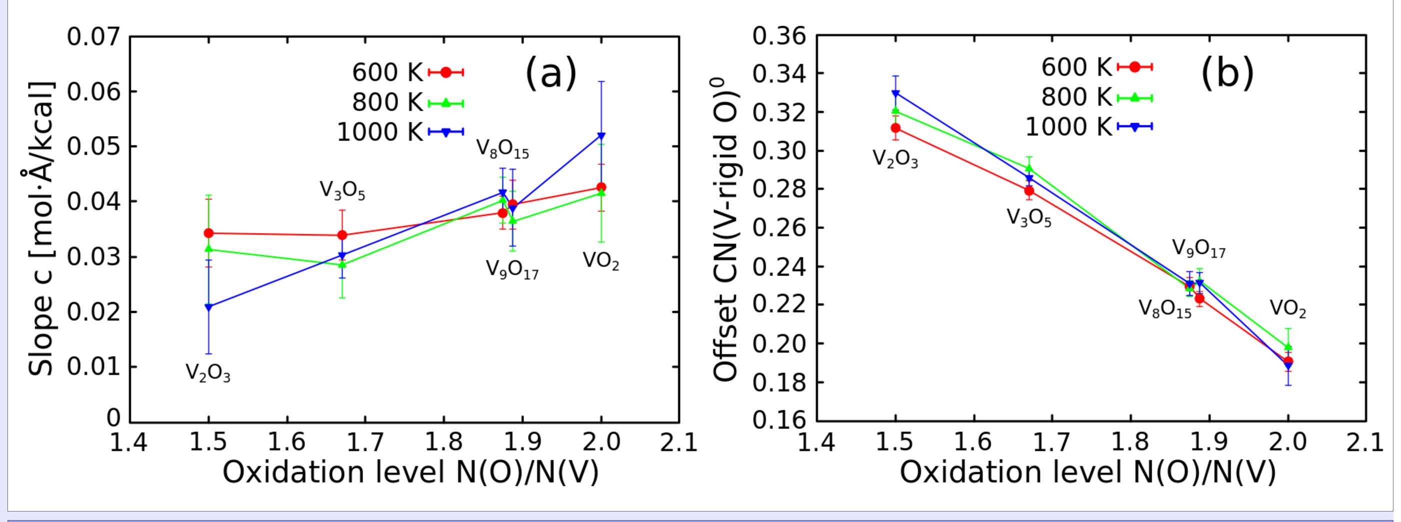


Slopes and offsets



$$F_x = COF \cdot F_z + F_x^0$$

$$CN(V-O) = c \cdot F_z + CN(V-O)^0$$



Conclusions

- Reactive molecular dynamics (reaxFF) simulations of the tribological properties of five selected VxOy done. All vanadium oxides were amorphous, which is a favourable structural characteristic, since they can provide liquid lubrication with a considerably low friction coefficient (COF).
- Friction coefficient COF increases with temperature and it weakly depends on stoichiometry.
- Our study of VxOy lubricants provides a reliable reference which is relevant for the development of hard and oxidation-resistant coatings containing vanadium as a doping lubricious element.

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