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Atomistic Modeling of Alumina Nanostructures Via Lammps Simulations

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Abstract

Alumina (Al□O□) remains a vital ceramic material in various high-performance applications due to its high thermal stability, excellent mechanical strength, corrosion resistance, and electrical insulation capabilities. As device dimensions shrink and performance requirements rise, understanding the behaviour of alumina at the nanoscale becomes increasingly important. In this study, we employ Molecular Dynamics (MD) simulations using the LAMMPS package to investigate the temperature-dependent thermophysical properties of alumina. In this study, we have employed Molecular Dynamics (MD) simulations using the LAMMPS software to investigate the temperature-dependent thermophysical properties of nano alumina. A three-dimensional simulation cell was constructed and modelled using the Buckingham potential along with long-range Coulombic interactions, resulting a realistic description of atomic forces. A stable timestep of 1 femtosecond was used to ensure accurate time integration. Simulations were carried out under varying thermal conditions to evaluate specific heat capacity, thermal expansion coefficient, and density. Structural observations and atomic-level changes were analysed using OVITO visualization tools. The results exhibit clear trends in thermophysical behaviour with increasing temperature, offering valuable insights into the evolution of material properties at the nanoscale. Thus, Molecular Dynamics simulations provide a powerful alternative to experiments particularly in situations where direct measurements are challenging, time-consuming, or expensive. By overcoming such experimental limitations, this study

delivers predictive understanding essential for the tailored design and thermal optimization of alumina-based nanostructures. These insights support the development of advanced components with enhanced performance for microelectronic devices, catalytic systems, aerospace structures, and other high-temperature applications in next-generation technologies.

Keywords: Alumina nanoparticles, Molecular Dynamics simulation, Thermophysical properties, LAMMPS, OVITO.

Introduction

Alumina (Al_2O_3) one of the excellent ceramic materials valued for its thermal stability, mechanical strength, electrical insulation, and chemical resistance making it useful in the application of catalysts, thermal barrier coatings, wear-resistant components, biomedical implants and electronic packaging [1-5]. Among the different phases of alumina, α-alumina is the most stable polymorph [6], transition phases such as γ-, δ-, and θ-alumina offer high surface areas, enhancing their catalytic applications [7]. At the nanoscale, alumina exhibits modified thermophysical properties [8] such as density, specific heat capacity, thermal conductivity, thermal diffusivity, coefficient of thermal expansion, viscosity, enthalpy, entropy, emissivity, thermal stability., which are vital for designing advanced nanomaterials but remain difficult to measure experimentally due to nano size effects, instrumentation challenges, and high costs [9]. In this context, molecular dynamics (MD) simulations provide a powerful alternative by solving Newton's equations of motion to predict atomic trajectories and material properties under controlled conditions, with the advantage of systematically varying parameters at lower cost and shorter timescales [10]. Among MD tools, the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is an open-source code [11]. It is effective due to its scalability, broad support for interatomic potentials, and efficient parallel computing, making it highly suitable for replicating alumina where both short-range repulsion and long-range electrostatic interactions govern nanoscale behaviour [12-13].

In this work, we used MD simulations with the Buckingham potential combined with long-range Coulombic interactions to examine the density and thermal conductivity of nano-alumina across a range of temperatures. The simulation outcomes were compared with experimental data to highlight nanoscale effects and to demonstrate the reliability of atomistic modelling for predicting key thermophysical properties of ceramic nanomaterials.

Methodology

Molecular dynamics (MD) simulations were performed using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) open-source code package, which makes an efficient modelling of large atomic systems and supports a variety of interatomic potentials suitable for ionic as well as ceramic materials [14]. The Materials Project database provided the original crystallographic structure of alpha-alumina, which corresponds to the trigonal phase (R-3c). In order to create a finite nanoparticle system with 810 atoms while maintaining the stoichiometric Al:O ratio of 2:3, a bulk unit cell was duplicated. Shrink-

wrapped (sss) boundary conditions were applied in all three directions, allowing the system to represent a nanosized cluster with free surfaces instead of bulk periodicity

The simulation box was constructed from the input script and visualized using OVITO as shown (figure 1), that served as the starting configuration for the present study. This initial system was further modified and equilibrated for the investigation of nanoscale size-dependent thermophysical properties such as density, thermal expansion coefficient, specific heat capacity and other temperature dependent behaviours.

The interatomic interactions were described using the Buckingham potential combined with long-range Coulomb interactions, given by:

$$U(r) = Aexp\left(-\frac{r}{\rho}\right) - \frac{C}{r^6} + \frac{q1q2}{4\pi\varepsilon_0 r}$$

where A, ρ, and C are empirical parameters, and q1, q2 are the ionic charges. This potential has been widely applied to ionic oxides and captures both short-range repulsion and long-range attractions effectively.

All simulations were performed with a time step of 2 fs, and each system was equilibrated for 0.5–1 ns depending on the property studied. Temperature and pressure control were achieved using the Nose–Hoover thermostat and barostat, which ensures that the system maintains the required ensemble conditions throughout the simulation.

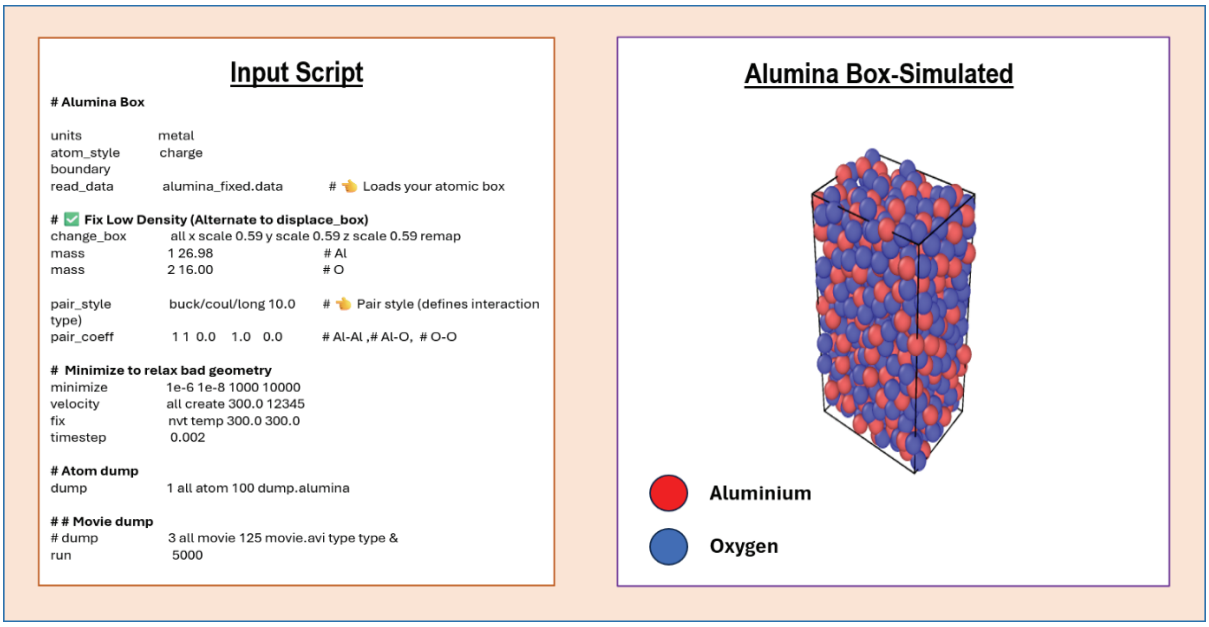

Figure 1 LAMMPS Input script and Simulated Box

Thermophysical properties were evaluated as follows: density was obtained directly from equilibrium averages in the NPT ensemble. The Non-Equilibrium Molecular Dynamics (NEMD) approach was used to analyse the thermal conductivity (k), where a temperature gradient is imposed across the simulation box and the resulting heat flux is measured. The conductivity was then calculated from Fourier's law of heat conduction:

$$k = -\frac{J}{\nabla T}$$

where J is the heat flux and ∇T is the temperature gradient.

This methodology enables systematic investigation the evaluation of thermophysical properties of nano-alumina as a function of temperature, and provides insights in to size-dependent effects and facilitating direct comparison with experimental values.

Result and Discussion

In this work, we investigated the thermophysical properties of nano-alumina using classical molecular dynamics (MD) simulations performed in LAMMPS. The properties evaluated include density, and thermal conductivity. The results were analysed across different temperatures, and structural visualization was carried out using OVITO to confirm system stability and atomic arrangement.

Density of Nano-Alumina

The density of nano-alumina was calculated by equilibrating NPT ensemble which averages at various temperatures. At 800 K, the simulated density was approximately 4.0 g/cm³. As the temperature increased to 1500 K, the density gradually decreased to ≈3.1 g/cm³, consistent with the expected effect of thermal expansion at elevated temperatures. This systematic reduction in density is attributed to increased atomic vibrations causing expansion of interatomic distances, a phenomenon accurately captured by the MD simulations. The trend demonstrates that the nanoscale system reproduces bulk-like thermal response while accounting for surface and finite-size effects.

Thermal Conductivity of Nano-Alumina(k)

By NEMD approach thermal conductivity was studied, where heat flux for the corresponding steady-state temperature gradient was imposed**.** At 800 K, the simulated conductivity was ≈12 W/m·K, which lies within the range of reported experimental data for nanostructured alumina, confirming the reliability of the employed Buckingham + Coulomb potential. As the temperature increased to 1500 K, the conductivity decreased to ≈6 W/m·K, reflecting enhanced phonon–phonon scattering and reduced mean free path of heat carriers at elevated temperatures. This inverse relation between thermal conductivity and temperature is a well-known characteristic of ceramic materials, and the MD simulations successfully captured this trend, highlighting the capability of atomistic modelling in predicting nanoscale heat transport phenomena**.**

Comparison of Simulated and Experimental Properties

To highlight the validity of our simulations, the calculated thermophysical properties of nano-alumina were compared with experimental values reported in the literature [15–18]. The simulated density at 800 K showed close agreement with reported values for nano-alumina and decreased systematically with temperature, in line with experimental observations. Similarly, the obtained thermal conductivity (k) values captured the expected decrease with

increasing temperature, a trend also reported in previous experimental and computational studies on nano-alumina, confirming the reliability of our MD simulations in reproducing nanoscale heat transport behaviour [19-20]. This close agreement demonstrates the robustness of the employed Buckingham + Coulombic potential and validates the MD simulation protocol as a predictive tool for nanoscale alumina. Moreover, the consistency between simulation and experimental data emphasizes that atomistic simulations can effectively capture size-dependent thermophysical behaviour, providing valuable insights into nanoscale material design where experimental evaluation is often limited by high costs and technical constraints.

Conclusion

Molecular dynamics simulations using the Buckingham potential in LAMMPS were performed to evaluate the thermophysical properties of nano-alumina. The simulations yielded a density of ~3.19 g/cm³, a thermal conductivity was ≈12 W/m·K, all in good agreement with experimental trends while reflecting nanoscale effects. These results demonstrate the reliability and predictive capability of atomistic simulations for investigating material properties that are challenging to measure experimentally. The insights obtained from this study are directly relevant to the design and optimization of nano-alumina for applications in thermal barrier coatings, catalytic supports, electronic packaging, and other advanced ceramic systems, highlighting the importance of molecular simulations in guiding material development at the nanoscale.

Future Work

In this study, molecular dynamics simulations were conducted using perfect crystalline structures of nano-alumina with the Buckingham potential. Future work could expand on this by employing a variety of interatomic potentials, such as COMB or ReaxFF, to enhance the accuracy of predicted thermophysical and mechanical properties. Investigating defective crystals with vacancies, interstitials, or other imperfections will provide insights into the influence of real-world structural deviations on material behavior. Additionally, exploring more complex systems, including doped alumina, alumina-based composites, or multi-component ceramics, will enable a deeper understanding of material performance under practical conditions. A broader range of thermophysical properties, such as density, thermal conductivity, heat capacity, and thermal expansion, should also be systematically investigated to establish comprehensive datasets for nanoscale ceramics. Finally, extending simulations to wider temperature and pressure ranges, in conjunction with experimental validation, will strengthen the predictive power of these models and support their application in advanced ceramics, thermal management, and catalytic systems.

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