Proceedings of the 11th World Congress on Mechanical, Chemical, and Material Engineering (MCM'25)
Paris, France - August, 2025
Paper No. HTFF 121
DOI: 10.11159/htff25.121

Optimization of Thermophysical Properties of Pyrochlore-type TBCs Based on Molecular Dynamics Simulation

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Extended Abstract

$La_2Zr_2O_7$ (LZ) is a ceramic material with a pyrochlore-type structure, recognized for its excellent high-temperature stability and low thermal conductivity[1,2], which make it an ideal candidate for thermal barrier coatings (TBCs). However, its relatively low thermal expansion coefficient and fracture toughness limit its performance under extreme conditions. To further enhance its properties, this study employs machine learning (ML) potentials to investigate the thermal and mechanical properties of Ce^{4+}-doped $La_2(Zr_{1-x}Ce_x)_2O_7$ systems (x = 0, 0.125,0.25).

In the initial phase, training data were obtained through first-principles calculations using VASP[3,4],. The essential electronic and structural information was derived from these calculations and subsequently utilized to train the machine learning potential. The DeePMD-kit [5] was employed to train the ML model, which was subsequently applied in molecular dynamics (MD) simulations performed with LAMMPS [6]. This approach facilitates a more systematic and efficient investigation of the material properties across various doping concentration.

The results from the simulations indicate that increasing the Ce^{4+} concentration leads to an increase in the thermal expansion coefficient of $La_2(Zr_{1-x}Ce_x)_2O_7$. This increase is attributed to changes in the lattice structure induced by the Ce^{4+} doping concentration. The lattice constant modification enhances the thermal expansion behavior. Additionally, the higher Ce^{4+} doping concentrations promotes phonon scattering within the material, which in turn reduces the thermal conductivity. This reduction in thermal conductivity improves the thermal insulation performance, making it more suitable for high-temperature applications.

The application of the ML potential in this study demonstrates several advantages in simulating the properties of complex materials. It provides an efficient computational framework for exploring the structure-property relationships of $La_2(Zr_{1-x}Ce_x)_2O_7$, allowing for the simulation of larger systems and longer timescales than traditional methods. This method also facilitates a thorough analysis of the effects of Ce^{4+} doping on both thermal properties and mechanical properties.

The integration of ML and MD in this study advances the development of next-generation TBCs and high-performance materials. The use of ML potentials enables a more efficient investigation of the effects of doping on material properties, providing both theoretical insights and data to support the development of novel TBCs. This methodology offers a powerful tool for the optimization of ceramic materials for high-temperature applications, opening the door for the design of more efficient and durable TBCs. Moreover, this study offers a broader framework for advancing the development of advanced materials across various domains of materials science.

This study highlights the ML potential in accelerating the discovery and optimization of advanced materials, specifically in the context of TBCs. The combination of ML and MD allows for a deeper understanding of the underlying material behaviors and offers a pathway to the development of next-generation materials with enhanced properties. The findings presented in this study contribute to the expanding body of knowledge in material design and offer valuable insights for developing TBCs and related materials.

References

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