Thermal barriers for NextGeN turbine blades

Computational search for more efficient thermal barrier coatings using the Wigner formulation

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In Short

- Thermal barrier coatings (TBCs) play a pivotal role in the field of aerospace engineering, where they are used e.g. to protect the turbine blades of jet engines from thermal stresses and degradation;
- The durability and reliability of jet engines strongly depend on the thermal and mechanical properties of TBCs. Understanding which materials offer the best performances is an active area of research that is facing several challenges: experiments on these materials are time consuming and expensive, while theoretical studies based on molecular dynamics simulations have a high computational cost and do not directly provide information about the microscopic properties of the heat carriers;
- This project will explore the quantum, microscopic physics underlying the thermal transport in rare-earth(RE) zirconates and their solid solutions using the recently developed Wigner formulation and first-principles calculations, i.e. an approach which allows to resolve with quantum accuracy how every microscopic heat carrier contributes to heat conduction, and has much reduced computational cost compared to molecular dynamics simulations;
- This study will aim at understating how the interplay between anharmonicity and structural or chemical disorder determines the thermal conductivity, thus it will potentially lead to the development of novel design strategies for materials for TBCs.

Turbine blades of jet engines, electricity generators, and spacecraft are subjected to high-temperature air-flow damage. Thermal barrier coatings are employed to protect the base alloy of turbine blades under such a harsh environment. It is critical to improve the thermo-mechanical performance of TBCs for prolonged service life and to improve the efficiency of the components [1][2]. The ultimate goal is to develop materials with ultra-low thermal conductivity ($\leq$ 2 W/mK) and stability at high temperatures.

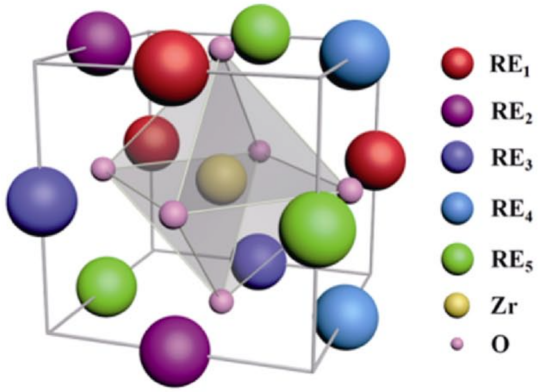

Figure 1: *Crystal structure of a zirconate containing multiple RE elements, taken from Ref. [6]. As a starting point, this study will focus on solid solution with chemical composition* $(La_{1-x}Yb_x)_2Zr_2O_7$.

Understanding the microscopic physics underlying thermal transport is crucial in developing the TBC material, which is prohibitively difficult through experimentation. From the theoretical front, standard molecular dynamics simulations have a high computational cost and offer limited insights on the microscopic physics, as they do not directly provide information about the microscopic, quantum properties of the heat carriers. Moreover, this problem cannot be tackled using the established microscopic Peierls-Boltzmann formulation for thermal transport. In fact, materials with ultralow thermal conductivity display a high-temperature decay milder than the T^1 trend observed in crystals where third-order anharmonicity is the dominant limiting factor for heat conduction. These limitations have been overcome with the recently introduced Wigner formulation of thermal transport [3][4]. This formulation has shown that particle-like and wave-like heat-conduction mechanisms have a comparable strength when the phonon interband spacings become comparable to the anharmonic linewidths, the so-called ”complex crystal” regime, typical of materials with ultralow or glasslike conductivity. Thus, the Wigner formulation will provide an accurate description of thermal transport in complex crystals and disordered materials [3][4][5]. In this project, we combine the Wigner formulation with first principle calculations to search for more efficient thermal barrier materials.

Rare-earth (RE) zirconates have a complex crystal structure, hetero-bonding, a large number of phonon bands and strong anharmonicity, making them po-

tential candidates for TBC applications [2].

As a starting point, this project will characterize the thermal transport in $La_2Zr_2O_7$ and $Yb_2Zr_2O_7$, two members of the RE-zirconate family. Then, the project will focus on studying thermal transport in their solid solutions, $(La_{1-x}Yb_x)_2Zr_2O_7$, studying compositions with variable degree of disorder ($x = 0.2, 0.4, 0.6, 0.8$). The work will be a pioneering effort in understanding how interplay between disorder and anharmonicity affects thermal transport in complex crystals, and in using state-of-the-art density-functional theory techniques to accurately describe solid solurtions containing RE elements. The harmonic and anharmonic force constants will be computed using the supercell approach using a synergistic combination of Quantum Espresso and hiPhive or ShengBTE packages. In addition, the frequencies and linewidths obtained from these force constants will be used to simulate the Raman spectrum using the dedicated workflow recently implemented in AiiDa; whenever possible these simulations will be compared with experiments to validate the accuracy of the theoretical approach employed. The thermal conductivity will be calculated using the linearized form of the Wigner transport equation (LWTE) implemented in the Phono3py code, where the scattering operator will be computed for the isotopic-mass disorder and anharmonicity. The unsolved theoretical question tackled in this proposal could potentially unveil the microscopic physics underlying thermal transport in solid solution with variable degree of disorder. In addition, the research proposed here will have a direct impact on TBC technologies. We aim to propose quantitative guidelines for engineering thermal transport in materials for thermal barriers via e.g. alloying.

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More Information

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