Thermophysical, electrical, and optical properties of $ZrC_{0.88}$ near melting from DeepMD

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We calculate the density, enthalpy, electrical resistivity, and spectral emissivity of zirconium carbide $ZrC_{0.88}$ near melting using molecular dynamics (MD) with a first-principles-trained neural-network potential. Training configurations were generated with a pretrained MACE foundation model and evaluated by density functional theory with the PBEsol exchange–correlation functional in VASP, providing energies, forces, and stresses. These data were used to fine-tune the pretrained DPA4-Neo-OMat24 model in DeepMD. MD simulations at different temperatures and densities yielded pressure and energy data used to reconstruct the 1-bar isobar in the solid and liquid phases around the experimental melting temperature of 3840 K. At melting, the calculated density decreases from 5.90 to 5.31 g/cm^3, corresponding to an approximately 11% increase in volume. The enthalpy of fusion is 131 kJ/mol, compared with the experimental value of 115.6 ± 12.0 kJ/mol for nearly stoichiometric zirconium carbide [1]. Kubo–Greenwood calculations give a decrease in electrical resistivity from approximately 287 to 212 $\mu\Omega \cdot$ cm upon melting. Experimental data for $ZrC_{0.95}$ also decrease from 290 ± 20 to 250 ± 20 $\mu\Omega \cdot$ cm [2]. At 905 nm, the calculated normal spectral emissivity decreases from 0.484 to 0.417, close to the experimental decrease from 0.50 to 0.43 reported for $ZrC_{0.98}$ [3]. The work is supported by the Russian Science Foundation (project No. 26-19-00980).

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[2] Савватимскии А И *et al.* 2022 *УФН* **192** 642–662

[3] Фролов А М 2021 *Исследование молекулярного состава паров сверхтугоплавких веществ методом лазерного испарения* Ph.D. thesis