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Thermodynamic and segregation analysis of oxygen vacancies in the 5 [001] CSL SrTiO3 twist grain boundary from first-principles[1]

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We studied the sigma-5 (001) SrTiO3 (STO) twist grain boundary (GB) using first-principles DFT calculations. We modeled three types of GB terminations, SrO-SrO (SS), SrO-TiO2 (ST), TiO2-TiO2 (TT), and studied their thermodynamic stability. We found that the SS and ST GB terminations are more energetically favorable than the TT GB termination. Oxygen vacancy formation in the GB structures was found to be more favorable than in bulk STO. Oxygen vacancy segregation energies were also calculated in the SS and ST GBs, to evaluate the preferred vacancy positions in these systems. In the SS system, oxygen vacancies exhibited a strong tendency to segregate to the SrO layers at the GB, rather than the grain interior. The reverse behavior was found in the ST system, where oxygen vacancies exhibited a strong tendency to remain within the TiO2 layers of the grain rather than segregate to the GB. To compare oxygen vacancy formation energies for each system on the same scale, we also calculated absolute oxygen vacancy formation energies for various vacancy positions in the SS and ST GB structures, along with that of bulk STO. Our results revealed that oxygen vacancy formation in both the SS and ST twist GB structures is substantially easier than in bulk STO.

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