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Surface Effect on the Half-Metallic and Thermoelectric Properties of Co_2TiSn [001] Film

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Received: April 2, 2020
Revised: April 2, 2020
Accepted: April 5, 2020

The half-metallic, mechanical, and thermoelectric properties of the Co_2TiSn in bulk and [001] films were investigated based on density functional theory (DFT) and full-potential linear augmented plane waves plus local orbitals method (FP−LAPW + LO). The exchange-correlation functional was approximated by generalized gradient approximation (GGA). The Co2TiSn bulk has mechanical stability in three static, dynamic, and elastic forms. All phonon branches have positive frequencies, and elastic results have shown the hardness with brittle behavior for this case. The Co_2TiSn has half-metallic nature with full spin polarization at the Fermi energy and $2.0\,\mu_B$ magnetic moment. It also has a good figure of merit (ZT) about one that makes it suitable for thermoelectric applications.

All four Co−Co, Co−Sn, Ti−Sn, and Ti−Co terminations of the [001] films have the ground state point. However, the Ti−Sn termination has half-metallic property so that in the up-spin it is metal and in the down-spin it is a semiconductor with an indirect energy gap of 0.3 eV. The thermoelectric behavior of the Ti−Sn termination has shown big Seebeck coefficient (S) with a positive sign and in lower temperatures, and the ZT amount around one in this temperature range. Moreover, the power factor (PF) of this case has a significant peak in the room temperature.

Keywords: DFT, Co_2TiSn film [001], half-metallic, thermoelectricity.