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Low resistivity contacts to thin film thermoelectric materials¹ CATALIN D. SPATARU, YUPING HE, FRANCOIS LÉONARD, DOUGLAS L. MEDLIN, Sandia Natl Labs, PHILIP BARLETTA, Micross Advanced Interconnect Technologies, NICHOLAS BALDASARO, DOROTA TEMPLE, Research Triangle Institute — Thin films of telluride materials such as Bi₂Te₃ and Sb₂Te₃ have been of interest for thermoelectric applications and for devices based on their topological insulator properties. In both cases, electrical contacts play a key role in determining performance, but little is known about the detailed properties of such contacts and ways to reduce the contact resistivity. Here, we employ a combination of ab initio and macroscopic simulations to establish the basic physics of these contacts and to establish realistic limits on the contact resistivity. We show that the nature of the semiconductor material leads to unusual contact properties, such as a strong interfacial atomic dipole, that completely determine the band-bending and strong n-type doping near the interface. We predict that significant improvements over previously reported experimental data are possible, and we present new experimental data that demonstrate a 100-fold reduction in contact resistivity. Detailed analysis of the new contacts shows that additional improvement should be possible. Importantly, we show that the reduction in contact resistivity can be harnessed to improve the thermoelectric efficiency of thermoelectric modules.

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Catalin D. Spataru Sandia Natl Labs

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