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Investigations of Interfacial Structure in Thermoelectric Tellurides

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At Sandia National Laboratories we are actively researching advanced thermoelectric materials to understand the mechanisms underpinning performance and long-term stability. A core area of our work is the investigation of internal interfaces since these can strongly affect the electronic and thermal transport processes controlling thermoelectric performance. In this presentation, I will discuss examples from our work investigating the atomic structure of interfaces in thermoelectric tellurides. I will begin by discussing the precipitation of tetradymite-structured plates within rocksalt-structured tellurides. Our electron microscopic observations of the $AgSbTe_2/Sb_2Te_3$ [1,2] and $PbTe/Sb_2Te_3$ [3] systems have identified how interfacial line defects can mediate the precipitation of tetradymite-structured Sb_2Te_3 plates within a rocksalt-structured matrix. Our analysis of the geometric properties of these defects clarifies the atomic rearrangements involved in the phase transformation and illustrates the interplay between the step geometry, misfit strain accommodation, and interface morphology. I will also discuss our analysis of the (0001) basal twin boundary in Bi_2Te_3 [4]. In the perfect bismuth telluride structure, the basal planes are arranged in a repeating sequence of 5-layer wide $Te^{(1)}$-Bi-$Te^{(2)}$-Bi-$Te^{(1)}$ packets. Our electron microscopic observations show that the reversal of stacking at the Bi_2Te_3 twin occurs at the $Te^{(1)}$ layers. This result is in good agreement with *ab initio* calculations, which predict a strong energetic preference for terminating the boundary at this layer. The results also have implications for the twinning mechanism. In particular, our calculations predict an energetic barrier for reversing the stacking at the Bi layer, suggesting that the twins cannot form by the independent motion of individual twinning dislocations. Analysis of the alternative configurations for interfacial steps provides solutions to this quandary [5]. Finally, I will discuss other thermoelectric materials systems where exploring the relationships between line defects, coherency strain, and interfacial growth mechanisms would be fruitful.

References:
[1] D.L. Medlin and J.D. Sugar, *Scripta Materialia*. 62 (2010) 379-382. doi:10.1016/j.scriptamat.2009.11.028
[2] J.D. Sugar and D.L. Medlin, *Journal of Materials Science* 46 (2011) 1668-1679. doi:10.1007/s10853-010-4984-4.
[3] N.A. Heinz, T. Ikeda, G.J. Snyder, and D.L. Medlin, *Acta Materialia* 59 (20) (2011) 7724-7735. 10.1016/j.actamat.2011.08.043
[4] D.L. Medlin, Q.M. Ramasse, C.D. Spataru, N.Y.C. Yang, *Journal of Applied Physics 108* (2010) 043517. doi:10.1063/1.3457902.
[5] D.L. Medlin and N.Y.C. Yang, *Journal of Electronic Materials* (in press) (2011). doi: 10.1007/s11664-011-1859-7