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Energetics and Diffusion of Gold in Bismuth Telluride MICHAEL SHAUGHNESSY, Synopsys, NORM BARTELT, JONATHAN ZIMMERMAN, JOSH SUGAR, Sandia National Laboratories — We investigate experimentally and theoretically the long-term chemical and morphological stability of Au contacts on Bi_2Te_3 . Electron microscopy and energy dispersive spectroscopy experiments show that thermal annealing severely degrades the integrity of micron-thick Au films, eventually leading to their complete dissolution. To explain this result, we have used density functional theory to calculate defect formation energies and diffusion barriers of Au within Bi_2Te_3 . We identify an interstitial binding site consistent with previous reports of (rapid) anisotropic diffusion of Au in Bi_2Te_3 . We find, however, that substitutional Au has lower formation energies. We suggest that these substitutional defects may be active in our experiments and account for the relatively long time scale of the contact degradation.

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