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Metal-Insulator Transitions in Crystalline Phase Change Materials WEI ZHANG, RWTH Aachen , Germany, ALEXANDER THIESS, Forschungszentrum Jülich, Germany, PETER ZALDEN, RWTH Aachen University, Germany, RUDOLF ZELLER, PETER DEDERICHS, Forschungszentrum Jülich, Germany, JEAN-YVES RATY, University of Liege, Belgium, MATTHIAS WUTTIG, RWTH Aachen University and JARA, Germany, STEFAN BLÜGEL, Forschungszentrum Jülich and JARA, Germany, RICCARDO MAZZARELLO, RWTH Aachen University and JARA, Germany — Phase-change materials are capable of undergoing fast and reversible transitions between amorphous and crystalline phase upon heating and have been exploited in data storage applications based on the strong optical/electrical contrast between the two phases. Recently, compelling evidence for a metal-insulator transition (MIT) solely due to disorder has been observed in the crystalline PCM $Ge_1Sb_2Te_4$ (GST) and similar compounds: upon annealing at temperatures T below 548K, the system exhibits insulating behavior due to Anderson localization; at higher T, it shows metallic behavior. In contrast to the MITs observed in other systems such as P-doped Si, in GST correlation effects do not play a role and the MIT occurs at fixed stoichiometry. In this work, we present a Density Functional Theory study of this effect. We consider a set of very large models of GST containing one to several thousand atoms and different degree of disorder. We identify the microscopic mechanism that localizes the electron wavefunctions near the Fermi energy in the insulating phase: these states are localized inside regions having large vacancy consequent dissolution of these vacancy clusters. These results could help to develop new device based on multiple resistance states.

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