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Investigating Relaxation in Chalcogenide Using Reverse Monte Carlo Modeling ELIZABETH JUELFS, JORDAN TAYLOR, ROMAN GOLOVCHAK, ANDRIY KOVALSKIY, JUSTIN OELGOETZ, Physics, APSU — Non-oxide, chalcogenide glasses (ChG) are composed of a meta-stable network of covalent bonds. Over time, this network relaxes to a more thermodynamically favorable (yet still meta-stable) state, which leads to significant property shifts over time. The mechanism of this relaxation is not well understood. In an effort to illuminate this mechanism, neutron and high energy X-Ray diffraction studies have recently been carried out on glass samples spanning 20 years in age. These studies have been analyzed using a reverse Monte Carlo methodology (RMC). RMC uses structures generated from a random process to produce simulated experimental data, which is then compared to the available experimental data. Structures are kept or rejected based on a probability calculated from the C2 derived by comparing the simulated and experimental data. Statistical analysis can then be carried out on the retained structures. This poster will present the status of that analysis along with what we believe we know about the relaxation mechanism.

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