Materials World Network: Phase change materials for nanoelectronics: A combinatorial approach to mechanistic understanding

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An integrated, interdisciplinary and synergistically collaborative international team is formed to exploit the new technology of combinatorial materials exploration (CME) to address fundamental issues in the development and nanoscale understanding of amorphous/crystalline phase transitions for applications to semiconductor nanoelectronics. The team will explore the physics and materials science of the amorphous-crystalline transition in complex materials and develop and test new experimental and informatics protocols for CME. The US-based researchers will focus on development of new chalcogenide phase change materials for non-volatile memory, while the Japan-based researchers will focus on development of amorphous ternary metallic systems with reproducible and tunable work functions for nanoscale CMOS.

The scientific and technological goals for this project are:

- To develop a fundamental framework for amorphous-crystalline stabilization and transition relevant to future semiconductor device technologies;
- To elaborate new CME designs varying both composition and processing on single samples;
- To establish a combinatorial informatics protocol for data sharing among different institutions.

In addition to its scientific and technical goals, the collaboration aims:

- To establish an international hub for vibrant collaborations through CME,
- To facilitate information exchange on technological materials;
- To provide a new paradigm of materials exploration as an educational program for both senior undergraduate and graduate students.

Intellectual merit: The large resistance change upon rapid amorphization or re-crystallization of indium-selenide based materials makes them prime candidates for terabyte scale non-volatile memory; however, the current materials are not yet optimal. These complex materials exhibit intrinsic vacancies and multiple bonding environments in the crystalline phase, whose role in controlling the amorphous-crystalline phase transition will be explored in this project. Combinatorial materials exploration will be used to fabricate samples where film composition, thickness, interface structure, substrate temperature and/or other parameters are varied systematically with position; these CME library samples will then be fully characterized with spatially-resolved probes to correlate these parameters with structural, electronic and phase-change properties. This CME screening will both identify trends to build a predictive framework for future materials development and identify optimal materials for in-depth study and development. These detailed studies will lead both to new device materials and to enhanced understanding of nanoscale mechanisms underlying the amorphous-crystalline phase transition.

Broader impacts: Advancement of CME methodology will enable progress across a broad range of scientific and engineering disciplines with dramatic impacts on the society beyond the semiconductor industries. The interactive materials informatics infrastructure to be developed and refined will enable researchers to share materials libraries throughout the world in a multi-disciplinary environment. With representatives from academia, industry, and both a US and a Japanese government laboratory, this collaborative effort forms a microcosm of CME users across the nation and world to test and develop the interactive database. Our multi-venue and multidisciplinary team also forms a nucleus for new research and educational strategies to train future leaders for the workforce of tomorrow. By exposing students to different venues, graduates will make seamless transitions to the workforce with full understanding of employment options in these different environments as well as the ability to bridge both disciplines and cultures as they work at the interface between science and engineering in the development of new paradigms, new science and new technologies.