Heterostructural Semiconductor Alloys

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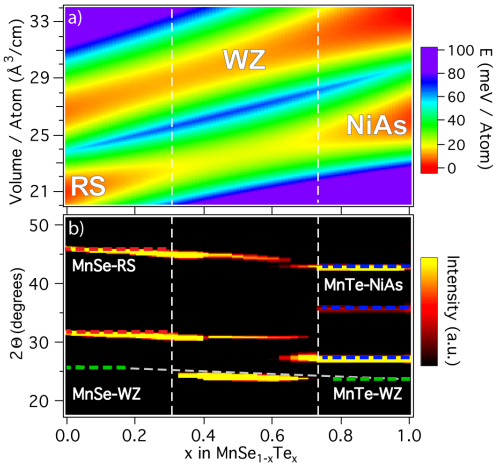
Solid solutions between two semiconductors with the same crystal structure are used to continuously tune the properties as a function of composition (e.g. GaN-InN), and are often referred to as "isostructural alloys". In the field of metallurgy, unique properties can be achieved by combing metals with different crystal structures, including high-strength superalloys, different forms of steel, high-entropy alloys, bulk metallic glasses, and other "heterostructural alloys".

In this presentation, I will discuss our recent research efforts in *heterostructural semiconductor alloys*, aimed to bring metallurgy ideas to the field of semiconductors. According to thermodynamics, composition-temperature phase diagrams of the heterostructural alloys should feature much wider metastable region where composition fluctuations are suppressed than in the case of isostructural alloys. Indeed, metastable (Mn,Zn)O thin films synthesized by high-throughput combinatorial physical vapor deposition validate this phase diagram and have optoelectronic properties that neither of the end-member MnO and ZnO compounds have.



The heterostructural alloying can also be used to synthesize wurtzite Mn(Se,Te) metastable polymorphs, which would otherwise require negative pressure to make. This unusual result can be explained by small bowing of mixing enthalpies that results from low interaction parameter of high-volume structures. The wurtzite-type Mn(Se,Te) alloys have properties that are markedly different from the parent NaCl-type MnSe and NiAs-type MnTe compounds, including piezoelectric response, wide optical bandgap, and low electron effective mass.

In summary, the results of this work demonstrate that heterostructural alloying ideas from the field of metallurgy can be used to design new semiconductors with useful properties.

Andriy Zakutayev is a scientist at National Renewable Energy Laboratory. Currently, Andriy is developing new materials for renewable energy technologies and studying the basic science of these materials, including oxides, nitrides, and sulfides. To achieve these goals, he applies combinatorial thin film physical vapor deposition methods, in close collaboration with computational scientists and advanced characterization experts. Andriy received his Ph.D. in Physics from Oregon State University, where he studied mixed-anion wide-bandgap p-type semiconductors for transparent electronics and solar cells.