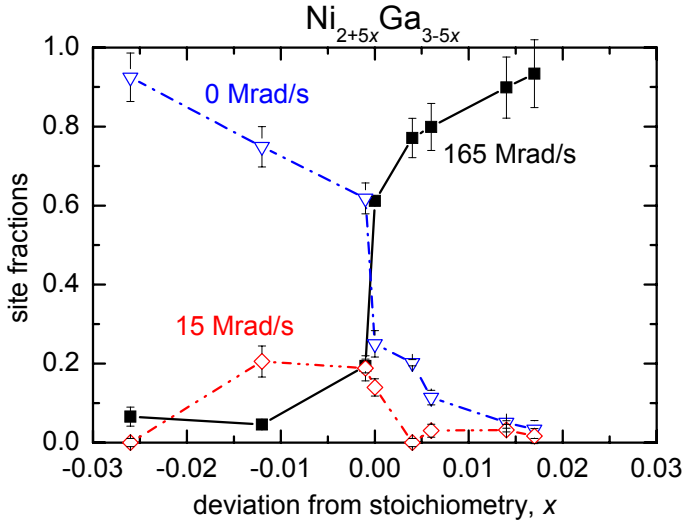
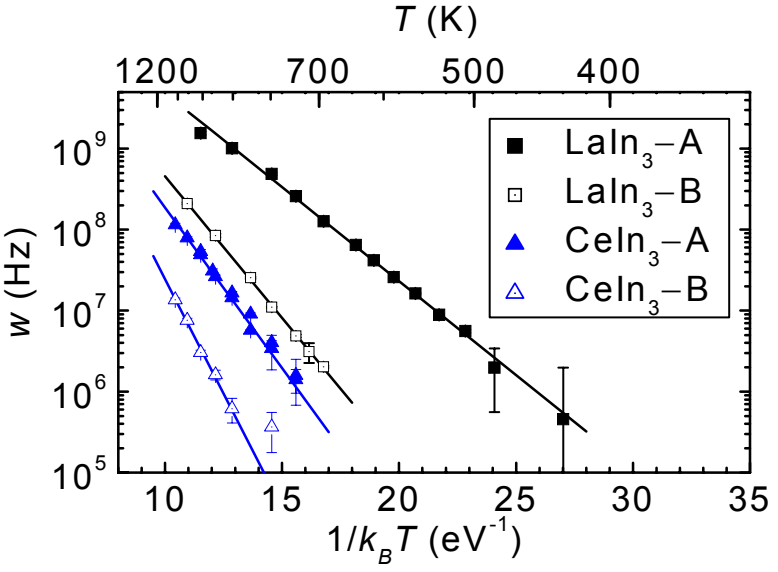
Nonstoichiometry in line compounds, Gary S. Collins, Washington State Univ., DMR 00-91681

Summary: A "line compound" has a precise composition at some stoichiometric ratio of elements. It is a useful construct in general even though, at finite temperature, all phases must have finite compositional ranges. However, properties highly sensitive to composition changes may vary significantly across the phase field in an unrecognized way. This can lead to unreproducible results, with largest differences generally expected for the two phase boundary (PB) compositions. This was recently demonstrated in our laboratory in measurements of two properties at opposing PB compositions, **(1) lattice location of solute atoms**, and **(2) jump frequencies of solute atoms at high temperature** (see below). Additional information in both cases suggested that the widths of the phase fields were only about 0.1 at.%.



Lattice location of In solutes in Ni_2Ga_3. Quadrupole interaction frequency changes from 0 to 165 Mrad/s for composition change much less than 1 at.% (0.01 on scale).



Jump frequency of solutes in two RIn_3 phases. Frequencies are 10-1000 times greater at more In-rich PB compositions (A) than less In-rich PB compositions (B).

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Significance

Researchers who study line compounds tend to overlook the possibility that some properties can vary significantly for composition changes as small as ~0.1 at.%. Our work shows that the differences can be large. To characterize properties sensitive to composition, we study two slightly two-phase samples in which compositions of the phase of interest are at the opposing phase boundary compositions. This provides two benchmarks for the property.

Education

Individuals contributing to these studies included three MS level graduate students at WSU, Li Kang, Denys Solodovnikov and Jipeng Wang, visiting graduate students Aurélie Favrot, from INSA, Rennes, France, and Egbert Nieuwenhuis, from the University of Groningen, The Netherlands. A senior contributor was Matthew Zacate, now Assistant Professor at Northern Kentucky University. Some group members and friends are shown at an informal get-together.

Further information

Physical Review Letters 92, 225901 (2004)
Physical Review B70, 24202 (2004)
Defect and Diffusion Forum 237-240, 195 (2005)
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http://defects.physics.wsu.edu/

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