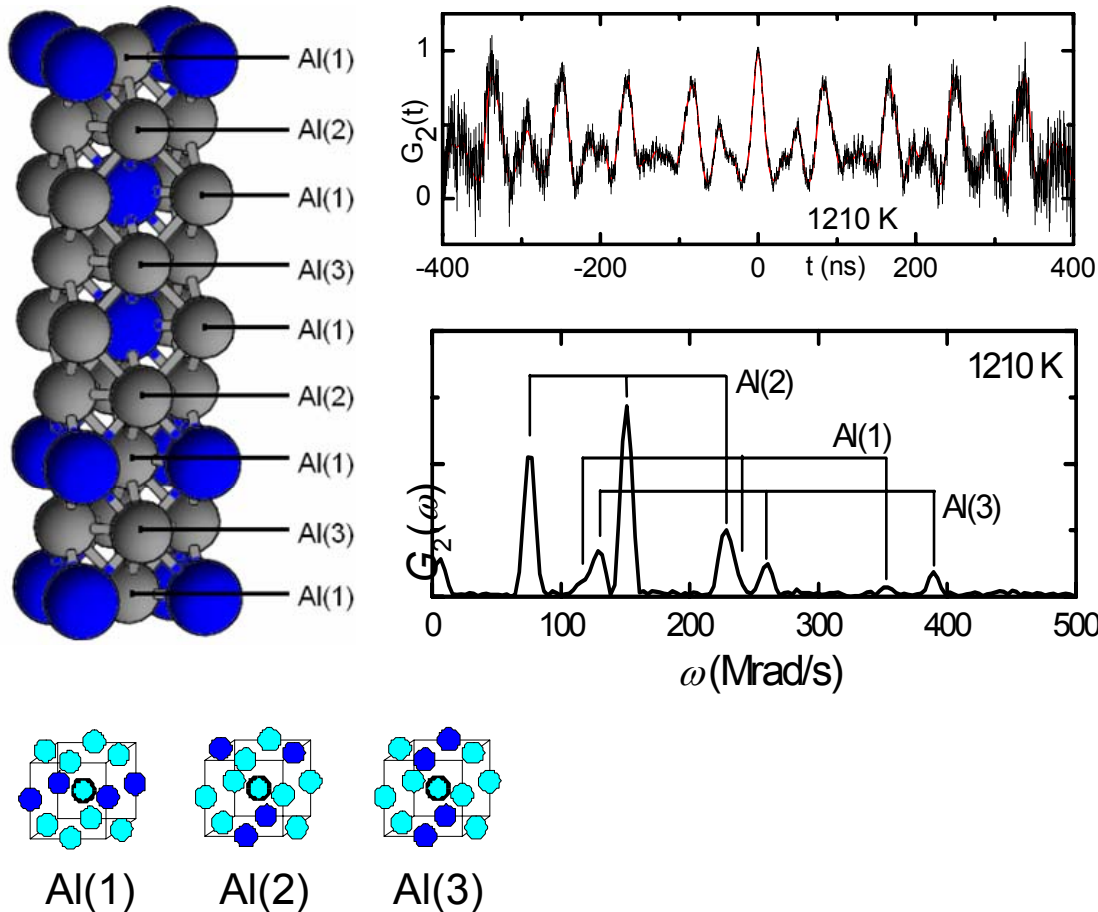


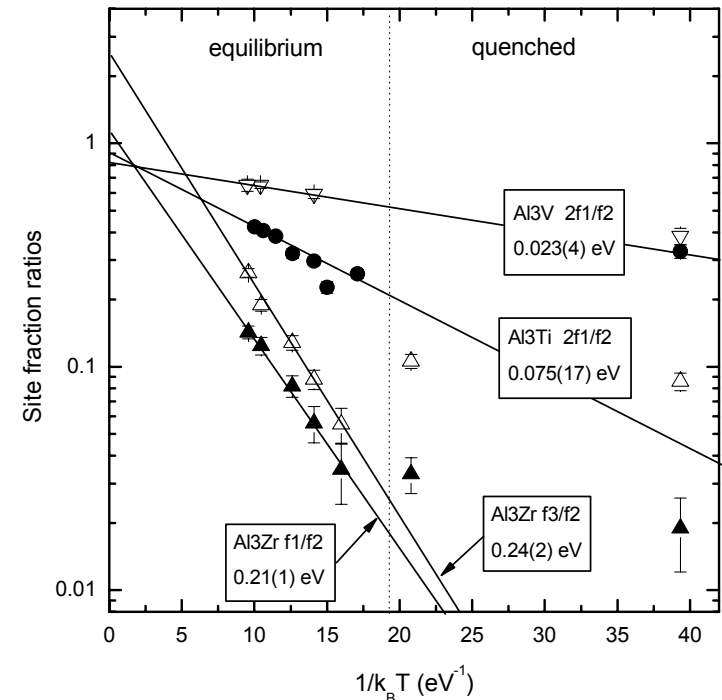
# Enthalpies and vibrational entropies of solutes in intermetallics

Gary S. Collins, Washington State University, DMR 05-04843

We measured site preferences of indium solutes among inequivalent Al-sites in phases having the  $\text{Al}_3\text{Ti}$  and  $\text{Al}_3\text{Zr}$  structures using the method of perturbed angular correlation of gamma rays (PAC). Sites were distinguished by measurements of nuclear quadrupole interaction frequencies. The diagrams show the crystal structure of  $\text{Al}_3\text{Zr}$  and local environments of sites Al(1), Al(2) and Al(3). Representative time and frequency spectra are shown from a measurement on  $\text{Al}_3\text{Zr}$  at 1210 K.



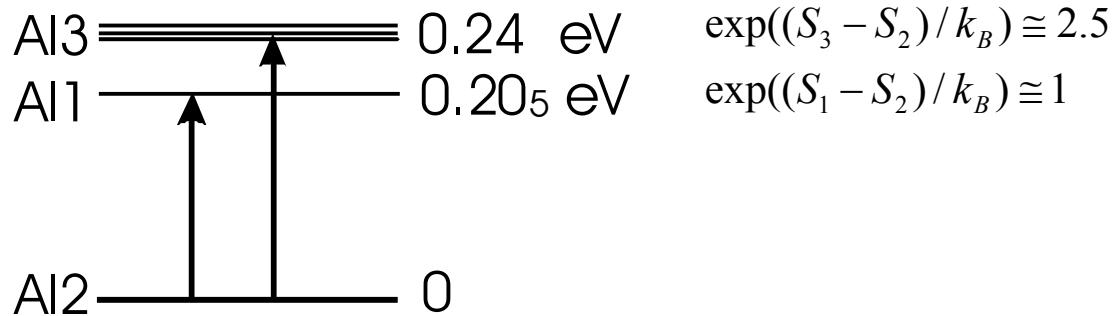
Below is an Arrhenius plot of site fraction ratios. Slopes give differences of enthalpies of indium solutes on pairs of sites. Intercepts at infinite-temperature give differences in vibrational entropies.



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From the Arrhenius plot, indium solutes in  $\text{Al}_3\text{Zr}$  can be seen to move among sites in a *three-state quantum system*, with degeneracies given by the entropy differences.



We are unaware of previous, comparable measurements. The precise values for enthalpies and entropies offer a challenge to be reproduced by condensed-matter computationalists.

Other impacts: Graduate student John Bevington and postdoctoral associate Farida Selim participated in these measurements. Preliminary results were presented at an conference in Brazil in August, with a fuller report to be submitted soon. This is just one project out of many under the grant. The recent photo at left shows seven research participants: three undergraduates, three graduate students and Farida (John is missing from the photo).



Research group in May 2007