

# Site preference of solute atoms in compounds

Gary S. Collins, Washington State Univ., DMR 00-91681

## Summary

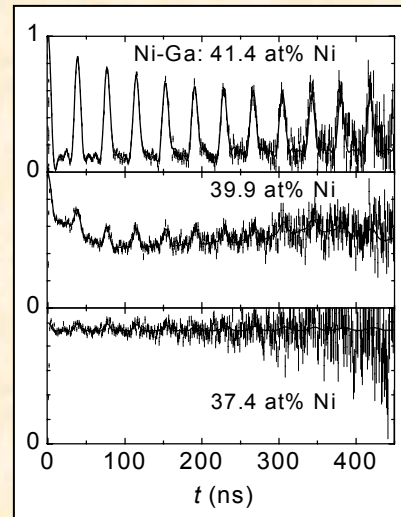
Preferences of solute atoms for different lattice sites in materials affect many properties. To study such preferences, we applied a hyperfine interaction method: perturbed angular correlation spectroscopy (PAC).

One can identify sites occupied by a dilute PAC probe solute by measuring nuclear quadrupole interactions that depend on local surroundings of the solutes.

We investigated the site preference of indium atoms present in two types of intermetallic compounds at very low concentrations (~10 ppb) and developed robust thermodynamic models to interpret the measurements.

Signals at different temperatures

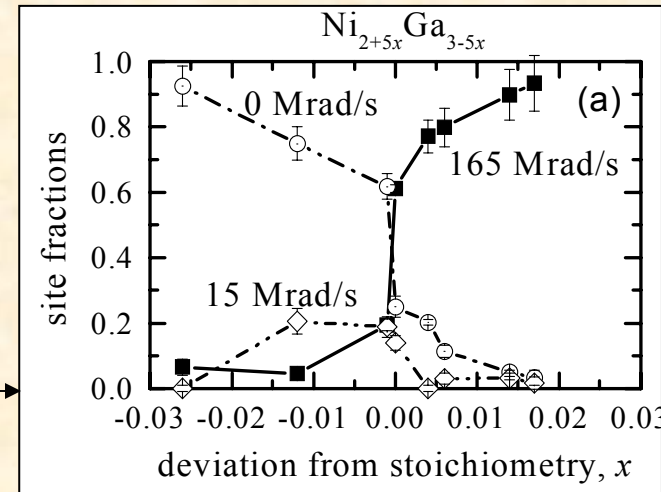
## Results for $\text{Ni}_2\text{Al}_3$ phases.



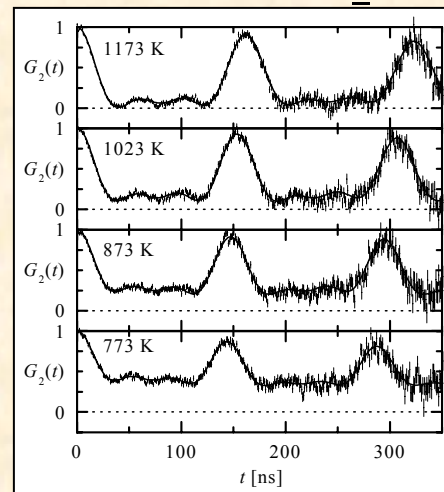
Signals at different compositions

Site fractions vary as a function of composition:

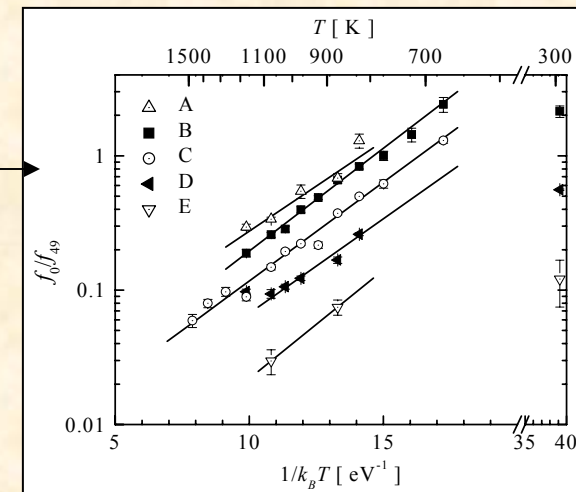
165= Ga-site  
0= Ni-site  
15= interstit. site



## Results for $\text{GdAl}_2$ .



Arrhenius plot of ratio of site fractions of signal for In on Gd-site (0 Mrad/s) and on Al-site (49 Mrad/s). Solute moves from Gd-site to Al-site with increasing temperature.



# Site preference of solute atoms in compounds

Gary S. Collins, Washington State Univ., DMR 00-91681

## Broad impact:

These are among the first studies of solute site preference undertaken with very dilute solutes. Thermodynamic models were developed by us to describe the phenomenology.

The studies show that the site preference is affected by temperature ( $\text{GdAl}_2$ ), and an activation enthalpy of 0.343 eV was determined for transfer of an In solute from the Gd to Al sublattice.

The studies on  $\text{Ni}_2\text{Al}_3$  phases (and on  $\text{GdAl}_2$ ) show that site preferences depend sensitively on composition near stoichiometric compositions. Moreover, site fractions were observed to be very different at the two phase boundaries of nominal “line” compounds of definite composition.

Experimentalists are cautioned that solute may “switch” sites even for very small differences of composition in “line” compounds.

## Dissemination of results:

An extensive report of results for  $\text{Ni}_2\text{Al}_3$  phases appeared recently in **Physical Review B70, 24202 (1-17) (2004)**, and includes heuristic rules to predict site selection behavior.

An extensive report of results for the phase  $\text{GdAl}_2$  appeared recently in **Physical Review B 69, 174202 (1-9) (2004)**.

## Education:

Measurements took place over a period of about 3 years, mostly carried out by Matthew Zacate, a postdoctoral associate and then research assistant professor supported by the grant. Matt Zacate recently accepted a permanent position at Northern Kentucky University.