

Site preferences of ^{111}In probe atoms in intermetallics having the Al_3Ti or Al_3Zr crystal structures

John P. Bevington,¹ Farida Selim,¹ and Gary S. Collins¹

¹*Department of Physics, Washington State University, Pullman, WA, USA*

Lattice locations of dilute $^{111}\text{In}/\text{Cd}$ probe atoms in phases having the Al_3Ti or Al_3Zr crystal structures were detected through measurements of nuclear quadrupole interactions using the method of perturbed angular correlation of gamma rays (PAC). The two structures are formed by stackings of Al-layers and mixed Al-T layers (T= transition metal) and are tetragonal. The Al_3Ti (or DO22) structure has one transition-metal site (T) and two inequivalent Al-sublattices having a 1:2 ratio of sites and designated Al(1) and Al(2). The Al_3Zr (or DO23) structure has one T-site and three inequivalent Al-sites having equal numbers of sites and designated Al(1), Al(2) and Al(3). T-sites in both structures are surrounded by 12 Al-atoms and accordingly were expected to have a very small electric field gradient (EFG). No such small EFG was detected. Local atomic environments of sites Al(1) and Al(2) are the same in both structures. The Al(1) site has four T-neighbors that form a square around the site whose normal is along the tetragonal axis and has a large EFG, whereas the Al(2) site has four T-neighbors in a distorted tetrahedral arrangement and therefore an EFG of intermediate strength. These expectations were supported by point-charge calculations of the EFG's at the different sites. Experimentally, it was found that ^{111}In probes strongly prefer Al(2) sites in all phases, with partial transfer of probes to Al(1) and Al(3) sites with increasing temperature.

When, as here, solute atoms are partitioned among inequivalent sites of a single element, it can be shown that the equilibrium ratio of populations is thermally activated with an activation enthalpy equal to the difference of site enthalpies [1]. As a consequence, for example, the ratio of site-fractions of probes on sites Al(2) and Al(1) in the Al_3Ti structure is

$$f_2/f_1 = 2 \exp((S_2 - S_1)/k_B) \exp(-(H_2 - H_1)/k_B T), \quad (1)$$

in which H_i and S_i are the enthalpy and vibrational entropy of the solute on the i^{th} site, and the factor 2 accounts for the different numbers of sites on the two sublattices. The above, very simple result does not apply when the two sites belong to different elements, as in our earlier studies [1][2]. Measurements were made of the temperature dependences of ratios of site-fractions in Al_3V , Al_3Ti and Al_3Zr . The data were fitted well with expressions like the one above, from which were obtained values of entropy and enthalpy differences between sites. Fitted enthalpy and entropy differences were in the ranges 0.02-0.25 eV and 0-1 k_B . Among other items to be discussed, it will be shown that the enthalpy differences are correlated linearly with differences in atomic radii of the T and Al atoms.

[1] Matthew O. Zacate and Gary S. Collins, Physical Review B70, 24202 (2004).

[2] Matthew O. Zacate and Gary S. Collins, Physical Review B69, 174202 (2004).

Email: collins@wsu.edu

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