Electric Field Gradient at Nb Site in the Intermetallic Compounds Nb_3X (X = Al, In, Si, Ge, Sn) Measured by PAC

A. C. Junqueira, A. W. Carbonari, J. Mestnik Filho, and R. N. Saxena Instituto de Pesquisas Energéticas e Nucleares – IPEN São Paulo, SP-Brazil Reprint requests to Dr. A. W. C.; Fax: +55(11)8169188, E-mail: Carbonar@net.ipen.br

Z. Naturforsch. **55 a,** 41–44 (2000); received August 25, 1999

Presented at the XVth International Symposium on Nuclear Quadrupole Interactions, Leipzig, Germany, July 25 - 30, 1999.

The electric field gradient (efg) at the Nb site in the intermetallic compounds N\\\\\\ X\ (X = Al, In, Si, Ge, Sn) was measured by the Perturbed Angular Correlation (PAC) method using the well-known gamma-gamma cascade of 133 - 482 keV in \(^{181}\)Ta from the \(\beta^-\) decay of \(^{181}\)Hf, substituting approximately 0.1 atom percent of Nb. The PAC results show that \(V_z\) drops by nearly 40% when X changes from Al to In, and by about 25% when X changes from Si to Ge and Sn. This behavior is most probably related to the change in the degree of sp hybridization in these compounds. The \(V_z\) values of the studied compounds do not follow the well known universal correlation for the efg's in non-cubic metals but the observed trend is well reproduced by results of ab-initio electronic structure calculations. In the case of \(Nb_3Al\) a linear temperature dependence of the quadrupole frequencies was observed in the temperature range of 6.5 to 1210 K.

Key words: Electric Field Gradient; PAC Measurements; Nb-based Alloys; Quadrupole Interactions.