

## Electronic contribution to electric field gradient in dilute alloys

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**Abstract.** A simple relation for calculating the electronic contribution to the electric field gradient in dilute alloys of transition metals is reported and is compared with the conduction electron charge shift model. The dependence of the field gradient on the *s* and *d* electrons and the difference in radii between the host and the probe atoms is considered for calculating the field gradient. It is found that the *d* electrons are the major contributors to the field gradient.

**Keywords.** Electric field gradient; electronic contribution; transition metals.

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### 1. Introduction

Measurement of electric field gradient (EFG) in metals using Mössbauer spectroscopy has been a field of active research for the past several years and theoretical calculations on the EFG have gained considerable attention in recent years. All the relevant charges contributing to the EFG are considered to be external to the nucleus. The field gradient in most cases is found to be amplified by the atomic electrons bounded by the nucleus. Theoretical calculations on the enhancement of the EFG by bound electrons have been done by Sternheimer (1966), Foley *et al* (1954) and Das and Bersohn (1956). The field gradient at the nucleus is written in the form:

$$eq = (1 - \gamma_{\infty})eq^{\text{ext.}} + (1 - R)eq^{\text{local}}. \quad (1)$$

The first term of (1) represents the field gradient arising from electrons and ions outside the atom or ion where the interacting nucleus resides, enhanced by the factor  $(1 - \gamma_{\infty})$ , where  $\gamma_{\infty}$  is the Sternheimer antishielding factor. Contributions to the field gradient due to the non-spherical unfilled orbitals of the atom are taken as  $(1 - R)eq^{\text{local}}$ ,  $R$  being the Sternheimer shielding factor, and represents the second term of (1). Equation (1) cannot be used as such to metallic systems and ionic solids (Beri *et al* 1978). The field gradient due to the lattice ions has been calculated considering the crystalline solids as an array of point ionic charges  $Ze$  situated at the lattice sites, where  $Z$  is taken to be the valence of the metal ion. The so-called ionic contribution ( $eq^{\text{ion}}$ ) written as  $(1 - \gamma_{\infty})eq^{\text{latt.}}$  is now used as the first term. Contributions from non-spherical electronic charge are presumed to represent an additional field gradient corresponding to the