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# SYSTEMATIC TIGHT-BINDING STUDY OF THE ELECTRON–PHONON INTERACTION IN METALS

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The electron–phonon interaction has been studied in the cubic transition metals using a tight-binding formalism. Accurate Slater–Koster fits to self-consistent, scalar-relativistic, augmented-plane-wave band calculations have been employed and scaling relations were used to determine gradients of the tight-binding matrix elements. Results for 3d and 4d transition metals are in agreement to within a few per cent with the rigid-muffin-tin calculations previously reported.

## 1. Introduction

An understanding of the electron–phonon interaction (EPI) in metals has been obtained by the rigid-muffin-tin approximation (RMTA) of Gaspari and Gyorffy (GG) [1] or from pseudopotential theory [2]. The RMTA has been used in a systematic study of the superconducting properties of cubic metals [3], and errors in the GG approximation (GGA) for light metals were accounted for in a study of the EPI by Zdetsis et al. [4]. For cubic transition metals the GGA appears to work well, although no independent checks have been done in a systematic way. In transition metal compounds, in hexagonal metals or in alloys, the RMTA equations of ref. 1 are more complicated to apply. The purpose of this paper is to present an independent check of theoretical calculations of the EPI in transition metals using a tight-binding approximation (TBA). This tight-binding approach has the advantage that it may be extended to hexagonal systems, alloys, and f electron systems without great difficulty.

## 2. Tight-binding formalism

The tight-binding formalism applied here is similar in spirit to earlier work [5–7] but differs in several details. The success of the present work depended upon the availability of very accurate electronic band structures of the elemental metals in a Slater–Koster representation [8], accurate numerical methods of performing Brillouin zone integration and a simple, systematic method of obtaining gradients of the potential matrix elements in the TBA.

The electron–phonon scattering matrix element between band $\mu$ at point $\boldsymbol{k}$ in the Brillouin zone and band $\mu'$ at point $\boldsymbol{k}'$ is [5]

$$g^{\alpha}_{\boldsymbol{k}'\mu',\boldsymbol{k}\mu} = \sum_{nm} A^{\dagger}_{\mu m}(\boldsymbol{k})[\gamma^{\alpha}(\boldsymbol{k}) - \gamma^{\alpha}(\boldsymbol{k}')]_{mn} A_{n\mu'}(\boldsymbol{k}') , \tag{1}$$

where $\alpha$ refers to $x$, $y$, $z$ components, $A_{\mu m}(\boldsymbol{k})$ is the eigenvector for band $\mu$, and

$$\gamma^{\alpha}_{lm}(\boldsymbol{k}) = \sum_{i} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i)\nabla_{R_{\alpha i}} \langle \Phi_{0l}|H|\Phi_{im}\rangle . \tag{2}$$

In the last equation $\Phi_{0l}$ is the $l$th atomic-like basis function located at the origin and $\Phi_{im}$ is the $m$th function located at position $R_i$ in a tight-binding

representation of the Hamiltonian, $H$, for the periodic solid. The EPI parameter $\langle I^2 \rangle$ is defined as the Fermi surface average,

$$\langle I^2 \rangle = \frac{\sum_{\alpha\mu\mu'} \int_{FS} \frac{d\sigma_{k\mu}}{|v_{k\mu}|} \int_{FS} \frac{d\sigma_{k'\mu'}}{|v_{k'\mu'}|} |g^{\alpha}_{k'\mu',k\mu}|^2}{\left[\sum_{\mu} \int_{FS} \frac{d\sigma_{k\mu}}{|v_{k\mu}|}\right]^2} . \quad (3)$$

Using transformation properties of the spherical harmonic orbital basis, eqs. (1)–(3) result in the simplified expression [7]

$$\langle I^2 \rangle = 2\left[\sum_{l} d_l A_l D_l - \sum_{mn\alpha} C^{\alpha}_{mn} C^{\alpha}_{nm}\right], \quad (4)$$

where

$$N(0) d_l A_l = \sum_{\mu} \int \left(\sum_{m} |A_{m\mu}|^2\right) \frac{d\sigma_{k\mu}}{|v_{k\mu}|} , \quad (5)$$

$$N(0) d_l D_l = \sum_{\mu\alpha} \int \left(\sum_{m} |\sum_{n} A_{n\mu} \gamma^{\alpha}_{nm}|^2\right) \frac{d\sigma_{k\mu}}{|v_{k\mu}|} \quad (6)$$

and

$$N(0) C^{\alpha}_{mj} = \sum_{\mu i} \int d\sigma_{k\mu} A^{*}_{m\mu} A_{i\mu} \frac{\mathrm{Im}[\gamma^{\alpha}_{ij}]}{|v_{k\mu}|} . \quad (7)$$

The integrals extend over the portion of the Fermi surface in the irreducible wedge of the first Brillouin zone. $N(0)$ is the density of states at the Fermi energy, $v_{k\mu}$ is the group velocity for band $\mu$ at point $k$ and $d_l$ is the dimension of the irreducible representation of the cubic group to which subset $l$ of the tight-binding basis functions belongs. For s, p and d electrons there are four subsets, so $l = 1, 2, 3, 4$ and $d_l = 1, 3, 3, 2$ for the usual ordering: $(s)$, $(x, y, z)$, $(xy, yz, zx)$, $(x^2 - y^2, 3z^2 - r^2)$.

## 3. Application to transition metals

Slater–Koster representations of the band structures of the cubic transition metals have been obtained by fitting self-consistent, scalar-relativistic, augmented-plane-wave (APW) calculations [8]. The orthogonal, two-centered version of the Slater–Koster method was employed in this work retaining first and second neighbor interactions in the tight-binding Hamiltonian. The typical rms deviation in these calculations was five mRy for the first six bands.

The scaling laws of Harrison [9] have been used to determine the gradients of the tight-binding Hamiltonian matrix elements in eq. (2). The advantage of the scaling laws lies in the fact that it is not necessary to have band structures at several lattice constants to calculate electron–phonon matrix elements. The scaling laws may be more reliable in estimating the gradients than band calculations at two lattice constants differing by a small amount because of the numerical sensitivity of the latter. In this scaling the ss, sp and pp bond parameters were varied as $R^{-2}$, the sd and pd as $R^{-7/2}$ and the dd as $R^{-5}$, where $R$ is the bond length [9].

The various Fermi surface integrals were evaluated using the analytic-tetrahedron method, including full variation of matrix elements throughout the zone. Tests of convergence of the integration grid size were made to insure accurate results for both face-centered and body-centered cubic metals.

No other approximations were made in the calculation. Group theory was used to avoid calculation of quantities which are zero, or equal to a previously computed quantity. In this way the calculations were made feasible for a large number of elements. Most of the computer time was spent evaluating the $C^{\alpha}_{mn}$ integrals, which contribute only a few per cent of the total in eq. (4). Details of the procedure are given elsewhere [11].

Results of the present calculation are shown in figs. 1 and 2 for 3d and 4d transition metals respectively, compared to the GGA results of ref. 3. All calculations were performed using cubic structures, non-cubic metals either omitted or done in a cubic phase. For transition metals agreement is quite satisfactory, as can be seen clearly in the figures, and supports the general

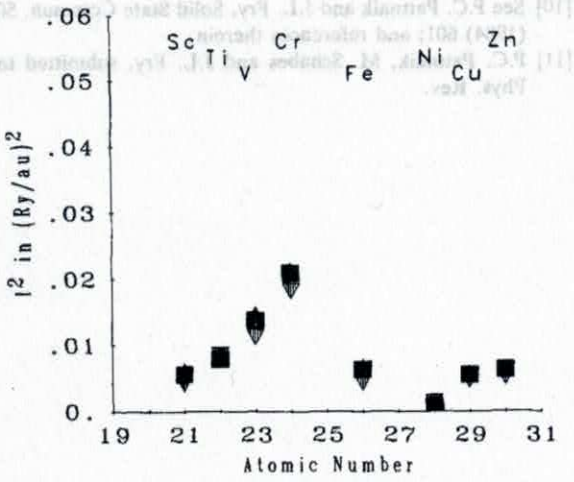


Fig. 1. $\langle I^2 \rangle$ in 3d transition metals. ▽ represents the GGA values from ref. 3; □ represents the TBA results neglecting the $C$ integrals in eq. (4); and △ represents the TBA results including the $C$ integrals.

validity of either GGA or TBA formulations of the EPI for these elements. Although both methods start with the same first principles band structures, the approximations made may be quite different. Incidentally, both methods, as expected, fail for simple metals unless corrected. The GGA underestimates and the TBA overestimates $\langle I^2 \rangle$ in simple metals unless corrections are made [4].

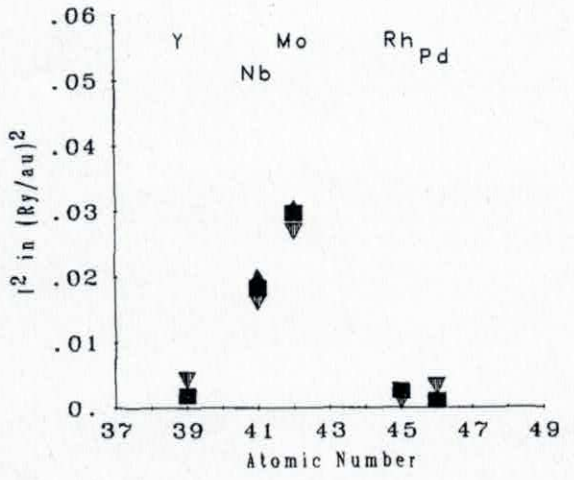


Fig. 2. $\langle I^2 \rangle$ in 4d transition metals. Symbols are the same as fig. 1.

## 4. Conclusion

A systematic study of the electron–phonon interaction has been presented within the tight-binding approximation for cubic transition metals, and a comparison with a parallel study of the EPI in which the RMTA theory of Gaspari and Gyorffy was employed. It is concluded that the two approaches are equivalent for the 3d and 4d transition metals, giving results which are in agreement to within a few per cent. Some of the differences may be due to the fact that the GGA results are based on non-relativistic band structure calculations whereas the Slater–Koster parameters were obtained from scalar relativistic band calculations for the heavier elements. This confirms the findings of previous work in a limited number of metals using a variety of approximations to make the calculations practical (see refs. 6 and 7, for examples). The validity of the tight-binding method opens up the possibility of studying superconducting parameters of hexagonal metals, transition metal compounds and alloys, and heavy fermion superconductors. These topics will be discussed in other publications.

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