ANNIHILATION MOMENTUM DENSITY OF POSITRONS TRAPPED AT VACANCY-TYPE DEFECTS IN METALS AND ALLOYS

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I. INTRODUCTION

Positron annihilation, especially the angular correlation of annihilation radiation (ACAR), is a powerful tool for investigating the electronic spectra of ordered as well as defected materials. The tendency of positrons to trap at vacancy-type defects should enable this technique to provide a signature of the local environment of such defects; an understanding of the changes in the defect structure at phase transitions is relevant also in the context of this conference. In order to achieve this goal, however, we need to develop a theoretical basis for calculating the two-photon annihilation momentum density $\rho_{2\gamma}(\vec{p})$. With this motivation, we have recently formulated and implemented a theory of $\rho_{2\gamma}(\vec{p})$ from vacancy-type defects in metals and alloys.[1] This article gives an outline of our approach together with a few of our results. Within the constraints of space, the discussion is mostly illustrative; the citation of literature is minimal.

An outline of this article is as follows. Section II summarizes the basic equations for evaluating $\rho_{2\gamma}(\vec{p})$. Our Green's function-based approach is non-perturbative and employs a realistic (one-particle) muffin-tin Hamiltonian for treating electrons and positrons; we are therefore able to handle ordered as well as disordered d-band systems. Section III presents and discusses $\rho_{2\gamma}(\vec{p})$ results for a mono-vacancy in Cu.[1] These are the first such results in a d-band metal; previous work has been limited to Al.[2] For simplicity, we have neglected the effects of electron-positron correlations and of lattice distortion around the vacancy in our implementation of the theory; further work to delineate these effects is required. Section IV comments briefly on the question of treating defects such as divacancies and metal-impurity complexes in metals and alloys.[3] Finally, in Section V, we remark on the form of $\rho_{2\gamma}(\vec{p})$ for a mono-vacancy in jellium.[4]
II. FORMAL CONSIDERATIONS

The starting point for the Green's function formulation of \( \rho_{2\gamma}(\vec{p}) \) is the equation:

\[
\rho_{2\gamma}(\vec{p}) = \frac{1}{\pi^2} \int d\vec{r} \int d\vec{r}' \exp[-i\vec{p} \cdot (\vec{r} - \vec{r}')] \int dE f(E) \int dE_+ f_+(E_+) \\
\times \text{Im} \, G(\vec{r}, \vec{r}'; E) \text{Im} \, G_+(\vec{r}, \vec{r}'; E_+),
\]

which expresses \( \rho_{2\gamma}(\vec{p}) \) in terms of the electron and positron Green's functions \( G(E) \) and \( G_+(E) \), and the associated Fermi-Dirac distribution functions \( f(E) \) and \( f_+(E) \) respectively. In the present application, it is useful to rewrite Eq. (1) in the form

\[
\rho_{2\gamma}(\vec{p}) = \sum_{mn} M_{mn}(\vec{p}) e^{i\vec{p} \cdot (\vec{R}_m - \vec{R}_n)}. \tag{2}
\]

Equation (2) decomposes \( \rho_{2\gamma}(\vec{p}) \) into a summation over the set \( \{\vec{R}_m\} \) of direct lattice vectors with matrix elements \( M_{mn}(\vec{p}) \).

A computationally tractable equation for the matrix elements \( M_{mn}(\vec{p}) \) is obtained by using the angular momentum expansion for the Greens' function within the KKR scheme:[5]

\[
\text{Im} \, G(\vec{r}_1, \vec{r}_2, E) = \sum_{LL'} Z_{L}^{(m)}(\vec{r}_1 - \vec{R}_m, E) \text{Im} \, T_{LL'}^{mn} \, Z_{L'}^{(n)}(\vec{r}_2 - \vec{R}_n, E), \tag{3}
\]

where \( \vec{r}_1(\vec{r}_2) \) lies in the Wigner-Seitz cell on the \( m(n) \) site, \( Z_{L}^{(i)} \) is the regular solution of the Schrödinger equation in the \( i^{th} \) muffin-tin sphere, and

\[
T(E) = [r^{-1} - B(E)]^{-1}, \tag{4}
\]

is the path operator matrix in the space of site indices \( n \) and the angular momenta \( L \). \( B \) is similarly a matrix which in a perfect crystal is the Fourier transform of the KKR structure constants, and the atomic scattering matrix \( r \) is related to the phase shifts of the individual scatterers. The use of expansion (3) for the electron and the positron Green's function straightforwardly yields the expression:

\[
M_{mn}^{\alpha\beta}(\vec{p}) = \frac{1}{\pi^2} \int dE f(E) \int dE_+ f_+(E_+) \sum_{L_1L_2} \sum_{L_1L_2} \Delta_{L_1L_2}^{n\alpha}(\vec{p}, E, E_+) \\
\times \Delta_{L_1L_2}^{n\beta}(-\vec{p}, E, E_+) \text{Im} \, T_{L_1L_1}^{mn}(E) \text{Im} \, T_{L_2L_2}^{mn}(E_+), \tag{5}
\]

where

\[
\Delta_{LL}^{n\alpha}(\vec{p}, E, E_+) = 4\pi \sum_{L''} (-i)^{n''} Y_{L''}(\vec{p}) \int d^3r \, Z_{L}^{n\alpha}(\vec{r}, E) Z_{L}^{n\alpha}(\vec{r}, E_+) Y_{L''}(\vec{r}) j_{n''}(pr). \tag{6}
\]

The superscript \( \alpha(\beta) \) in Eqs. (5) and (6) indicates that the site \( m(n) \) is occupied by atom of type \( \alpha(\beta) \); the superscript \( e(p) \) refers to electron(positron) quantities. The integration in Eq. (6) extends over the \( i^{th} \) cell volume \( \Omega_i \).