Pramāṇa – J. Phys., Vol. 30, No. 5, May 1988, pp. 435–442. © Printed in India.

Mass enhancement factor for Pd and Pt

A K BORDOLOI* and S AULUCK
Physics Department, University of Roorkee, Roorkee 247 667, India
*Permanent address: Physics Department, Jorhat Engineering College, Jorhat 785 007, India

MS received 25 September 1987; revised 28 January 1988

Abstract. We report calculations of the mass enhancement factors for Pd and Pt by comparing the physical quantities using the interpolation scheme band structure, with the corresponding experimental data. Our results are compared with other theoretical calculations.

Keywords. Band structure; Fermi surface; effective mass.

PACS Nos 71·38; 71·25

1. Introduction

In earlier papers we had reported calculations of the band structure and Fermi surface (FS) for Pd and Pt using the interpolation scheme where the parameters were chosen to fit the optical data as well as the FS extremal areas as measured by the dHvA experiments (Bordoloi and Auluck 1983a). It was shown that good agreement could be achieved if we define it in terms of a shift in Fermi level ΔE_F so that the calculated extremal area can be made to match with the experimental area. We find that extreme $\Delta E_F = 0{\cdot}0016$ Ry for Pt and 0·0022 Ry for Pd. We had also shown earlier that the calculated energy gaps at symmetry points (Bordoloi and Auluck 1983b) and $\varepsilon_2(w)$ (Bordoloi and Auluck 1988) were in good agreement with the experimental data.

In view of the success of our band structure in explaining the FS topology and the optical data, it would be interesting to calculate the dynamic properties of quasi-particles i.e. electron velocities $|\mathbf{v}_k^0|$, band masses m_b and density of states at the Fermi level $N(E_F)$. Comparison of these with the appropriate experimentally measured quantities yields three kinds of the enhancement factor. Our purpose here is to compare our calculated enhancement factor with other calculations and to see whether the enhancement factor obtained by the three different comparisons is consistent with each other.

Smith (1974) calculated the band structure of Pd and Pt using the combined interpolation scheme with the parameters chosen to fit the photoemission data obtained by him. Needless to say the agreement between this set of parameters and the experimental FS was rather poor (Bordoloi 1982). Hence the parameters were adjusted to obtain a good representation for the FS topology without destroying the agreement with optical data. This is referred to as our model, details of which are given elsewhere (Bordoloi 1982). Our model is so as to give a good agreement with optical data and FS geometry. We note in passing that with the interpolation scheme, which has numerous