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Asphericity in the Fermi Surface of d and f-Shell Metals

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<u>Abstract:</u> Recently proposed pseudopotential has been used to calculate asphericity in the Fermi surface of d and f-shell metals along the three symmetry directions [100], [110] and [111]. The parameter of the potential has been determined by zero pressure condition and the exchange and correlation function due to Taylor has been incorporated. The present results are in good agreement with experimental findings for Cu, Ag, Au and Pd; while for other d and f- shell metals we could not found sufficient theoretical as well as experimental data for the asphericity in the Fermi Surface in order to workout a quantitative comparison. It, therefore, seems difficult to give concrete remark about the present results. We conclude that the calculations of asphericity in the Fermi Surface based on pseudopotential theory can be regarded as a sensitive test for the proper assessment of the pseudopotential form factor. A successful application to the asphericity in the Fermi Surface confirms the ability of model potential for predicting wide range of physical properties of transition metals.

Key Words: Pseudopotential, Asphericity in the Fermi Surface, exchange and correlation effects

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