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Computational Study of Vibrational Dynamics of Binary $Mg_{0.70}Zn_{0.30}$ Metallic Glass by a Pseudopotential Theory

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Abstract: The vibrational dynamics of $Mg_{70}Zn_{30}$ metallic glass has been studied at room temperature in terms of phonon eigen-frequencies of longitudinal and transverse modes employing three different approaches proposed by Hubbard-Beeby (HB), Takeno-Goda (TG) and Bhatia-Singh (BS). The well-recognized model potential is employed successfully to explain electron-ion interaction in the metallic glass; instead of using experimental values of the pair correlation function g(r), which is generated from the computed pair potential. The present findings of phonon dispersion curve are found in fair agreement with available theoretical as well as experimental data. The thermodynamic properties obtained by HB and TG approaches are found much lower than those obtained by BS approach. The pseudo-alloy-atom (PAA) model is applied for the first time instead of Vegard's Law.

Key Words: Pair potential, Metallic Glasses, Phonon dispersion curves, Thermal properties, Elastic properties

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