Electron-Phonon-Interaction is an Intrinsic Parameter of Elements for Study Scattering and Search for New Materials

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The search of new superconducting, thermoelectric or dielectric materials has emphasized the importance of the dimensionless Electron-Phonon-Interaction (EPI) parameter λ. The critical temperature T_C is directly related with EPI by the McMillian formula [1]. When finding materials with large EPI they are also expected to have a large Seebeck voltage. In a previous investigation, we had found that EPI is correlated with rare earth dielectric properties and their Mendeleev number, when the elements are divided in groups of semi-conductors, transition, alkali and noble metals (Fig. 1 from [2]). While detailed EPI studies [3] are very time consuming, we provide here a new method. Electron-phonon interaction for about forty solid-state elements was analyzed by straining the crystal structure of a cubic unit cell of each chemical element in several steps in isotropic compression and expansion. The electronic band-structure is calculated by Vienna Ab-initio Simulation program (VASP). The stress dependences of seven bands below and above the Fermi level were analyzed for the different symmetry points, such as Γ, Δ, X, Z, M, Σ, Λ.

The results show that each element has a characteristic behavior like a fingerprint. Elements with a small EPI, like noble metals, show only weak strain dependences, or as a second type, all bands change in the same way. Elements with a large EPI show strong scattering of each symmetry points in a different manner (fig. 2 Nb, large EPI).

This new analysis method is a fast and useful tool for screening crystal structures whether they have a large EPI. The next step is applying to ternary phases [4].

[1] S. Y. Savrasov, D. Y. Savrasov, Phys. Rev. B 54 (1996) 16487-501

[2] W. Wunderlich, H. Ohsato, JJAP 52 (2013), doi: 10.7567/JJAP.52.09KH04

[3] W. Wunderlich, D. Menzel, Phonons in FeSi analyzed by ab-initio, Ann. Conf. German Physics Soc. (2011)

[4] W. Wunderlich, Y. Motoyama MRS. Symp. Proc. Vol. 1128-U01-10 (2009) 1-6.

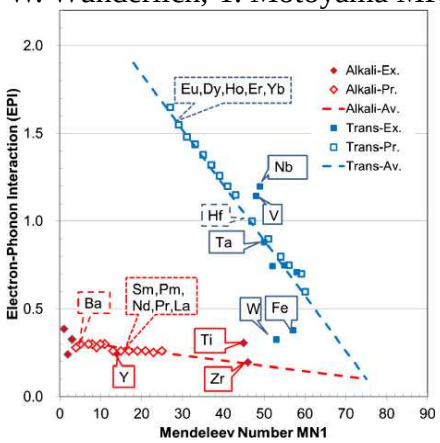

Fig. 1 Dependence of electron-phonon interaction on Mendeleev number MN1 [2]

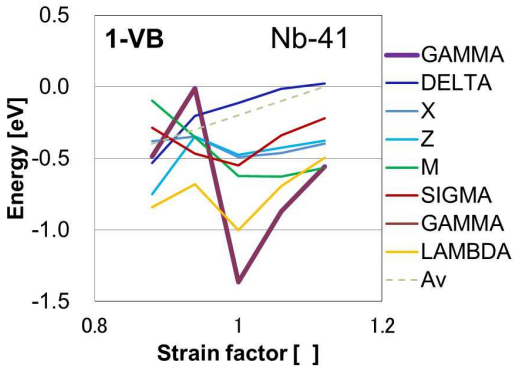

Fig. 2 Strain dependence of the energy of the first valence band in Nb (λ=1.25)