

## Supplementary Information

# Exploring finite-temperature electronic transport in CoSi alloys with transition metals (Cr, Mn, Fe, Ni) using the KKR-CPA method

Ho Ngoc Nam,<sup>\*a</sup> Quan Manh Phung,<sup>bc</sup> Katsuhiko Suzuki,<sup>d</sup> Hikari Shinya,<sup>efghi</sup>

Akira Masago,<sup>ik</sup> Tetsuya Fukushima,<sup>il</sup> and Kazunori Sato<sup>\*imn</sup>

<sup>a</sup>*Institute of Materials Innovation, Institutes of Innovation for Future Society, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8601, Japan*

<sup>b</sup>*Department of Chemistry, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*

<sup>c</sup>*Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8601, Japan*

<sup>d</sup>*Department of Mechanical Engineering, National Institute of Technology, Niihama College, Niihama, Ehime 792-8580, Japan*

<sup>e</sup>*Center for Spintronics Research Network (CSRN), The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

<sup>f</sup>*Department of Electrical Engineering and Information Systems, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

<sup>g</sup>*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

<sup>h</sup>*Center for Science and Innovation in Spintronics (CSIS), Tohoku University, 2-1-1, Katahira, Aoba-ku, Miyagi 980-8577, Japan*

<sup>i</sup>*Center for Spintronics Research Network (CSRN), Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan*

<sup>k</sup>*Research Institute for Value-Added-Information Generation, Japan Agency for Marine-Earth Science and Technology, Yokohama, Kanagawa 236-0001, Japan*

<sup>l</sup>*National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8560, Japan*

<sup>m</sup>*Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*

<sup>n</sup>*Spintronics Research Network Division, Institute for Open and Transdisciplinary Research Initiatives, Osaka University, Toyonaka, Osaka 560-8531, Japan*

\*Email: [honam@sp.material.nagoya-u.ac.jp](mailto:honam@sp.material.nagoya-u.ac.jp) (HNN); [ksato@mat.eng.osaka-u.ac.jp](mailto:ksato@mat.eng.osaka-u.ac.jp) (KS)

## The Change of Lattice Constants in Alloy Systems

It is known that doping or alloying foreign atoms into the host lattice could lead to significant changes in the lattice constants, thereby affecting the electronic structure of the system. Therefore, we have taken into account the effect of transition metals ( $X = \text{Fe}, \text{Cr}, \text{Mn}, \text{and Ni}$ ) alloying on the lattice constants of CoSi at different concentrations by using the linear fitting method (Fig. S1).

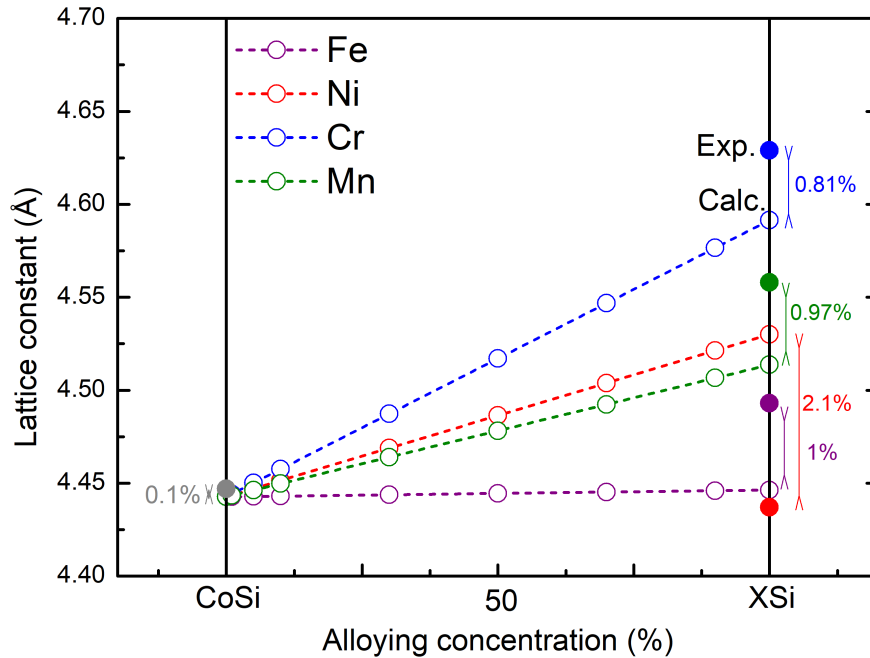


Fig. S1: Calculated lattice constants of alloys as a function of alloying concentrations, experimental data is included for comparison of the deviations (%). The calculated lattice constants of host lattice and foreign were found to be consistent with experimental data.<sup>1</sup>

## Phonon DOS and Atomic Displacement of Transition Metals

To estimate the influence of transition metals on the electronic states of the system, it is necessary to determine the displacement of each foreign atom. In this study, we estimated their atomic displacements based on their partial phonon

DOS (Fig. S2) in their respective alloys with Si (FeSi, CrSi, MnSi, and NiSi).

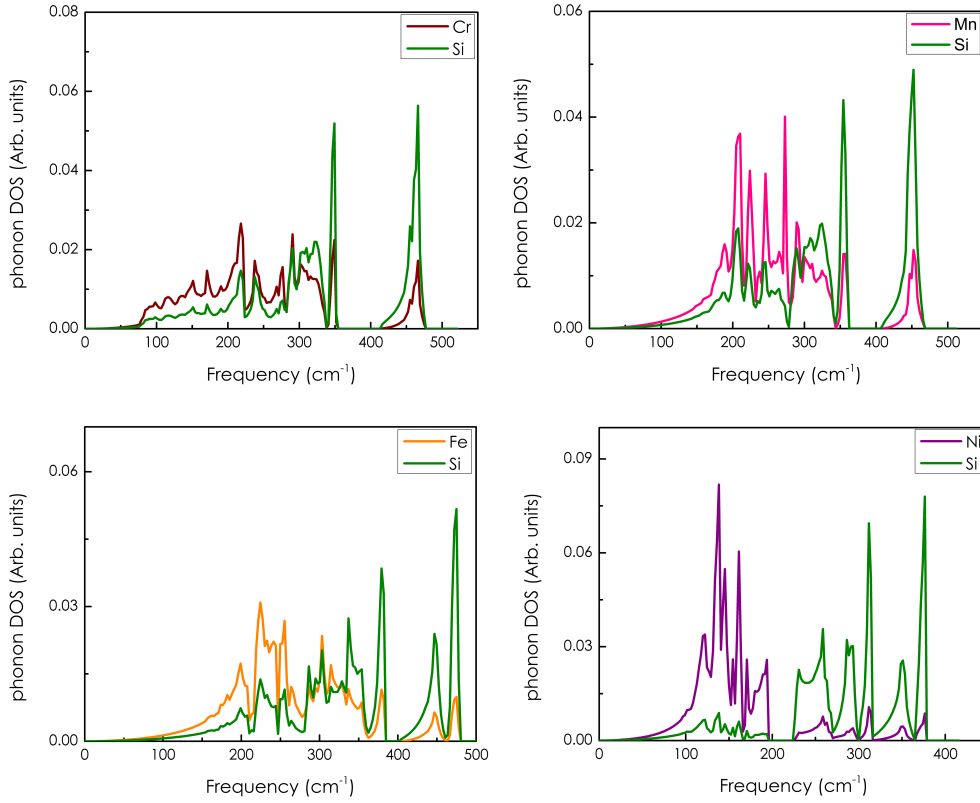


Fig. S2: The partial phonon DOS of Cr, Mn, Fe, and Ni in the compounds of CrSi, MnSi, FeNi, and NiSi, respectively.

## Effect of Anti-site Disorders on System's Resistivity at Different Concentrations

The effect of Co-Si antisite disorders on the system's resistivity is different with different concentrations (Fig. S3). At very small concentrations, we found that their influence on the conductivity is mainly dominant at low temperatures, then gradually diminishes in the high-temperature range. However, as their concentrations became significant, their influence in the high-temperature range gradually larger and could be equivalent to the contribution in the low-temperature range.<sup>2</sup>

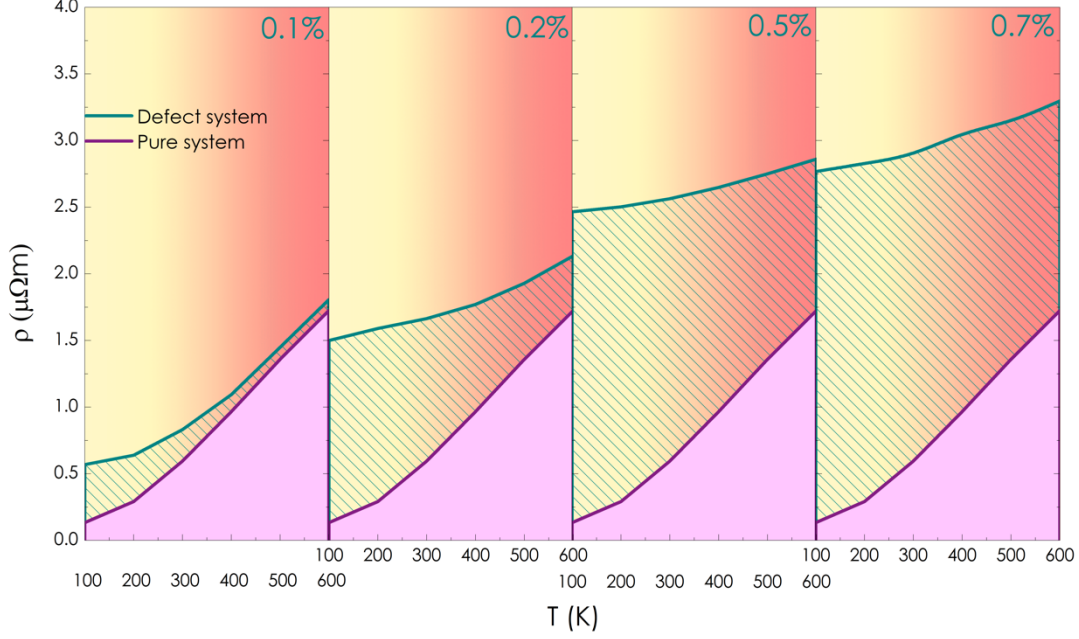


Fig. S3: Contribution of Co-Si anti-site disorders on the electrical resistivity of the system at different concentrations and temperature ranges.

## The contribution of vertex correction to the system's resistivity

Adding vertex correction is often associated with sophisticated theoretical methods for improving the accuracy of predictions related to electronic properties, especially electrical resistivity. In our work, we employed the Kubo-Greenwood formula for such calculations, where vertex functions are taken into account via ladder-like approximation.<sup>3</sup> In Fig. S4, the contribution of vertex correction on the resistivity of CoSi is elucidated by comparing the difference in resistivity before and after vertex correction is applied. We found that its influence in our system is quite small, only about a few  $\mu\Omega\text{cm}$ . Its effect was also found to be smaller at the low-temperature range and only becomes more significant at higher temperatures. Therefore, it can be pointed out that the reasonable treatment of scattering by local phonon displacement is primarily responsible for improved

prediction of system's resistivity at high temperatures, while vertex correction only has a minor effect.

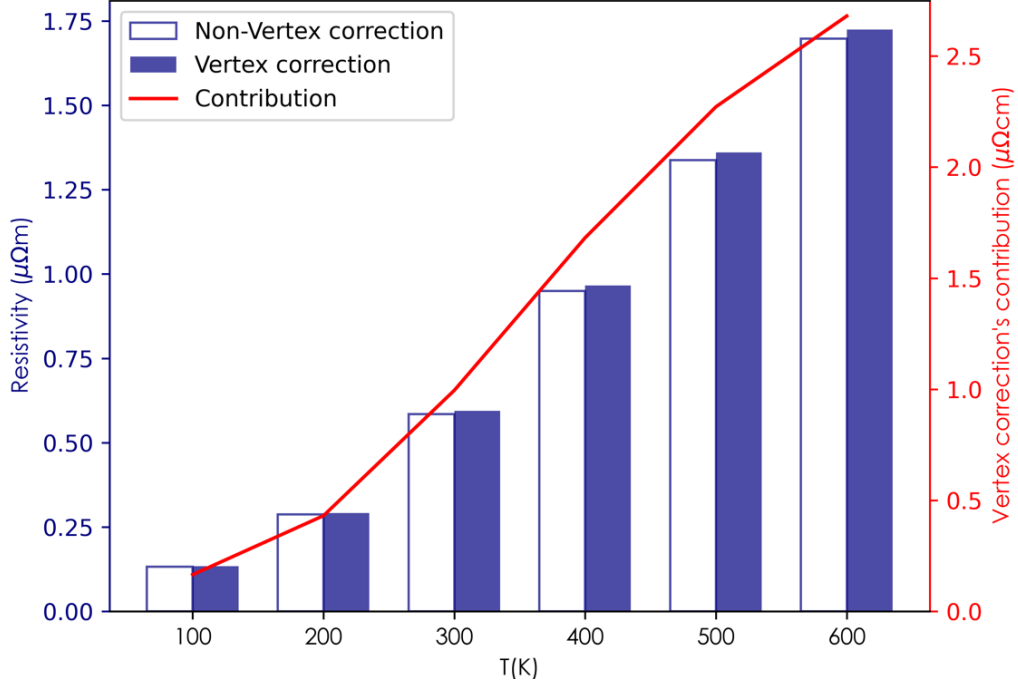


Fig. S4: The contribution of vertex correction on electrical resistivity of CoSi compound

## REFERENCES

- (1) D. Van der Marel, A. Damascelli, K. Schulte and A. Menovsky, *Spin, charge, and bonding in transition metal mono-silicides*, Physica B Condens. Matter, 1998, 244, 138–147.
- (2) H. Shinya, S. Kou, T. Fukushima, A. Masago, K. Sato, H. Katayama-Yoshida and H. Akai, *First-principles calculations of finite-temperature electronic structures and transport properties of Heusler alloy  $Co_2MnSi$* , Appl. Phys. Lett., 2020, 117, 042402.
- (3) W. H. Butler, *Theory of electronic transport in random alloys: Korringa-Kohn-Rostoker coherent-potential approximation*, Phys. Rev. B, 1985, 31, 3260.