Pressure dependence of Curie temperature and resistivity of complex Heusler alloys

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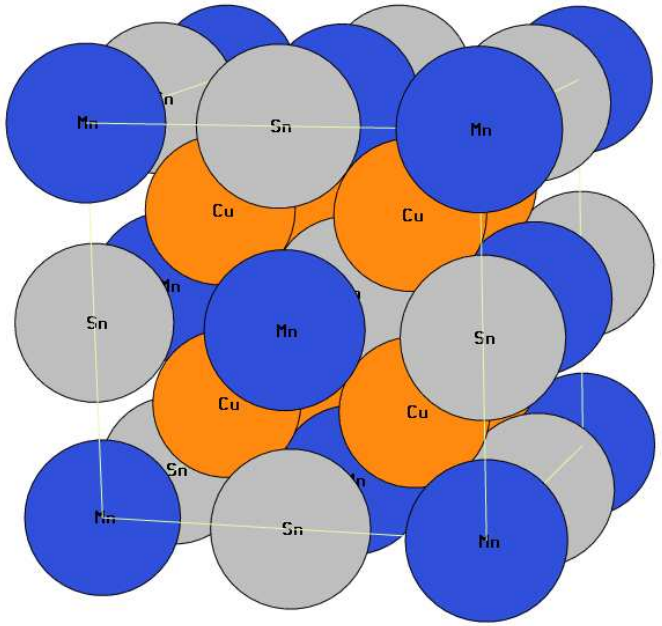


Heusler alloys $(Ni_xCu_{1-x})_2MnSn$ and $(Ni_xPd_{1-x})_2MnSn$

$L2_1$ structure

fcc lattice

$$\mathbf{A}_1 = a\left(0, \tfrac{1}{2}, \tfrac{1}{2}\right)$$
$$\mathbf{A}_2 = a\left(\tfrac{1}{2}, 0, \tfrac{1}{2}\right)$$
$$\mathbf{A}_3 = a\left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right)$$

basis

$\boldsymbol{\tau}_1 = a(0,0,0)$ ..... (Cu, Ni) or (Pd,Ni)
$\boldsymbol{\tau}_2 = a\left(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}\right)$ ... Mn
$\boldsymbol{\tau}_3 = a\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)$ ... (Cu, Ni) or (Pd,Ni)
$\boldsymbol{\tau}_4 = a\left(\tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{4}\right)$ ... Sn

MOTIVATION

- Heusler alloys have interesting physical properties and promising technological applications
  - magnetic shape memory
  - magnetocaloric effects
  - spintronics
- effects of high pressure:
  - increased electron kinetic energy
  - increased overlap of orbitals and band broadening
  - modification of Coulomb interactions
  - changes of Fermi surface
  - changes of magnetic moments and exchange interactions
  - changes of transport properties
- high pressure brings new information on the system
  - new degree of freedom
  - independent probe into physical properties
  - serves as a test of theory

OUTLINE

- ELECTRONIC STRUCTURE
- EXCHANGE INTERACTIONS
- CURIE TEMPERATURES
- TRANSPORT PROPERTIES
- DISCUSSION
- CONLUSIONS

ab initio study of Curie temperature under pressure for nonrandom Ni_2MnSn:
Sasioglu et al. Phys. Rev. B **71** 214412 (2005)

properties at ambient pressure:
Bose et al. Phys. Rev. B **82** 174402 (2010), J. Kudrnovský at DPG Dresden 2011

properties at high pressure:
Bose et al. Phys. Rev. B **84** 174422 (2011) and present contribution

ELECTRONIC STRUCTURE

TB-LMTO-CPA

xc: Vosko-Wilk-Nusair, experimental lattice constants

pressure is simulated by the reduction of lattice constant

3 % reduction corresponds approx. to 16 GPa in Ni_2MnSn

EXCHANGE INTERACTIONS 1

classical Heisenberg Hamiltonian

$$H^{\mathrm{Heis}} = -\sum_{ij} J_{ij}\, \mathbf{e}_i \cdot \mathbf{e}_j$$

$$\mathbf{e}_i = \frac{\mathbf{M}_i}{|\mathbf{M}_i|} \quad \ldots \text{ unit vectors}$$

exchange interactions ... J_{ij}

$J_{ij} > 0 -$ ferromagnetic coupling

$J_{ij} < 0 -$ antiferromagnetic coupling

magnetic force theorem: Liechtenstein formula: Liechtenstein et al. JMMM **67** 65 (1987), Turek et al. Phil. Mag. **86** 1713 (2006)

$$J_{ij} = \frac{1}{4\pi}\,\mathrm{Im}\int_C \mathrm{tr}_L\left[\Delta_i(z)\,\bar{g}^{\uparrow}_{ij}(z)\,\Delta_j(z)\,\bar{g}^{\downarrow}_{ji}(z)\right]\mathrm{d}z$$

$\Delta_i(z) = P_i^{\uparrow}(z) - P_i^{\downarrow}(z)$, $\bar{g}^{\sigma}_{ij}(z)$ ... intersite block of the Green function

EXCHANGE INTERACTIONS 2

exchange interactions between Mn atoms are calculated in the DLM state, then induced moments vanish

effects of high pressure:

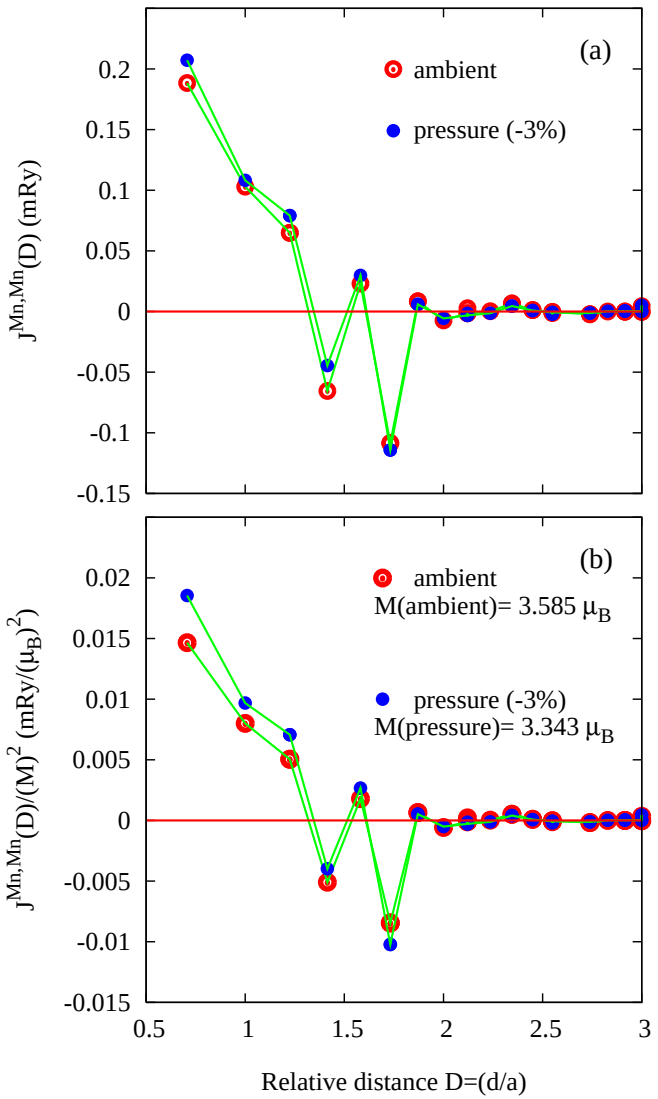
- diminished moments
- increased overlaps and thus exchange interactions are stronger

bare interactions

$$J_{ij}^{\mathrm{bare}} = J_{ij}/(M_i M_j)$$

$$H^{\mathrm{Heis}} = -\sum_{ij} J_{ij}^{\mathrm{bare}}\, \mathbf{M}_i \cdot \mathbf{M}_j$$

Ni_2MnSn



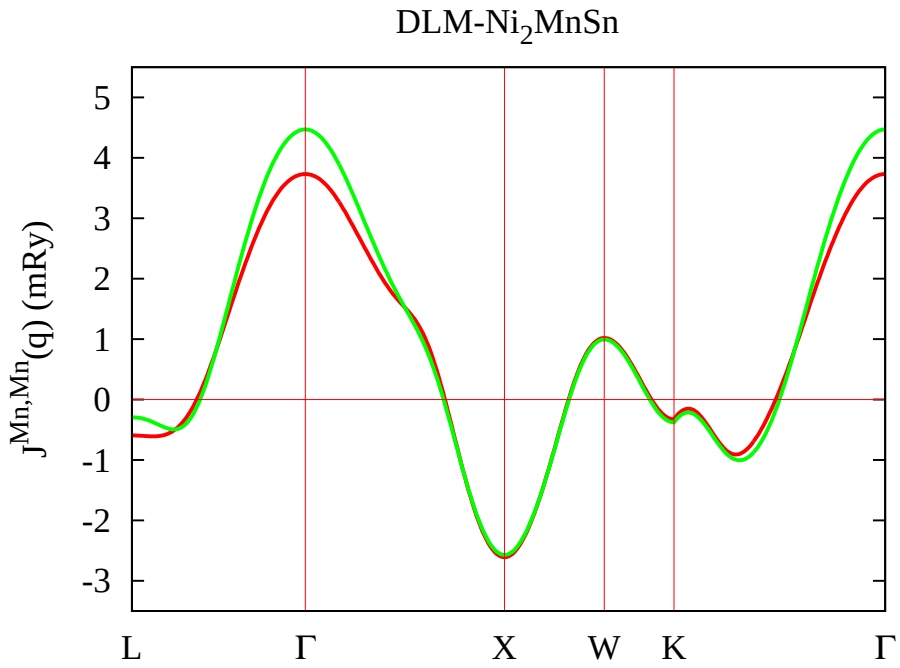
GROUND STATE

the ground state of systems with one sublattice is given by a single $\mathbf{q}$-vector wave which corresponds to the maximum of the Fourier transform of exchange interactions:

$$J(\mathbf{q}) = \sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j} J_{0,j}$$

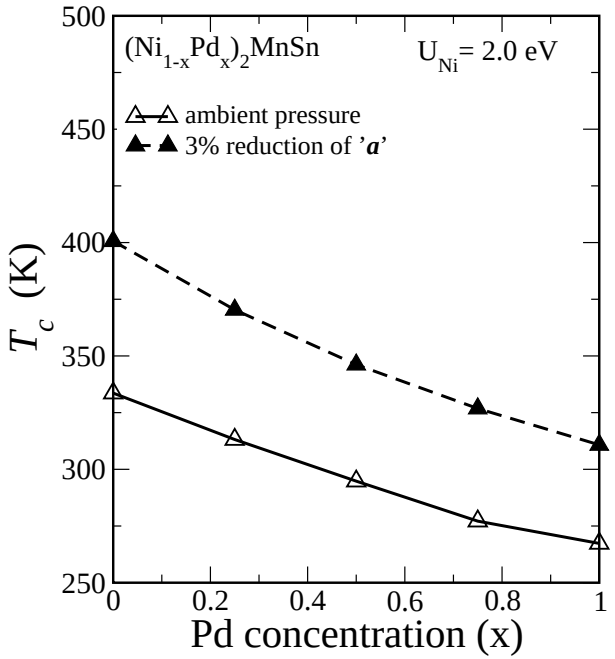
red line: ambient pressure
green line: high pressure (-3% a)
the ground state character is not changed

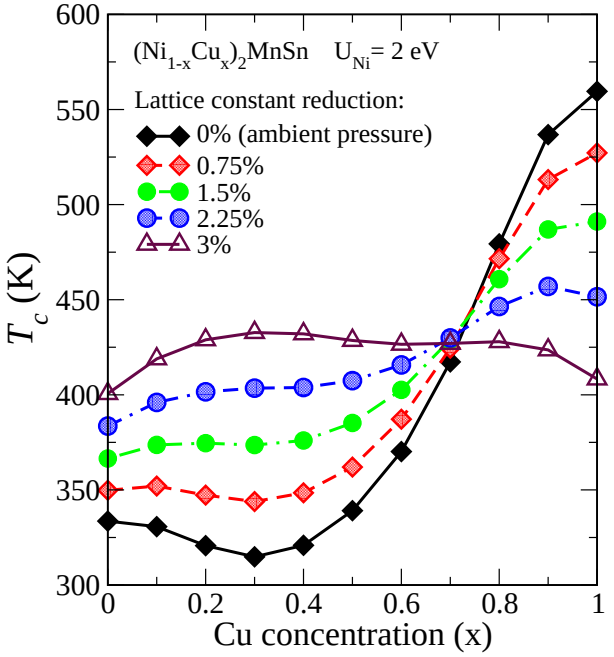
maximum at Γ-point: ferromagnet



CURIE TEMPERATURE 1

$$k_{\mathrm{B}} T_{\mathrm{C}}^{\mathrm{MFA}} = \frac{2}{3} \sum_i J_{0i} \,, \qquad \frac{1}{k_{\mathrm{B}} T_{\mathrm{C}}^{\mathrm{RPA}}} = \frac{3}{2} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{J(\mathbf{0}) - J(\mathbf{q})}$$





Curie temperature increases with pressure in $(\mathrm{Ni}_x\mathrm{Pd}_{1-x})_2\mathrm{MnSn}$ for all x and in $(\mathrm{Ni}_x\mathrm{Cu}_{1-x})_2\mathrm{MnSn}$ for $x < 0.7$ while it decreases in $(\mathrm{Ni}_x\mathrm{Cu}_{1-x})_2\mathrm{MnSn}$ for $x > 0.7$

CURIE TEMPERATURE 2

comparison with experiment:

data available for Ni_2MnSn and Pd_2MnSn shows increase of T_C with pressure
Austin, Mishra Phil. Mag. **15** 529 (1967), Gavriliuk et al. J. Appl. Phys. **79** 2609 (1999)

exchange mechanisms:

- direct exchange: not important as d(Mn-Mn) > 4 Å
- Anderson's superexchange (AFM): becomes stronger for smaller interatomic distances, tendency to lower T_C, might be important, but it does not explain behavior of Heusler alloys
- Stearns indirect exchange between localized and itinerant d electrons: analogy to RKKY, oscillatory (FM or AFM), necessary for explanation

delicate balance of superexchange and Stearns indirect exchange: only ab initio calculations can make quantitative prediction

TRANSPORT PROPERTIES

mechanisms responsible for resistivity in magnetic metals:

- scattering on static atomic disorder (impurities etc.): residual resistivity ρ_0
- scattering on lattice vibrations $\rho_{\rm vib}$
- scattering on magnetic disorder $\rho_{\rm mag}$

for simplicity assume that these mechanisms are independent: $\rho = \rho_0 + \rho_{\rm vib} + \rho_{\rm mag}$
individual contributions can be extracted from measured temperature dependence:

- residual resistivity $\rho_0 = const.$
- scattering on lattice vibrations $\rho_{\rm vib}(T) \propto T$ above Debye temperature (small)
- scattering on magnetic disorder $\rho_{\rm mag}(T) \propto T^2$ for $T < T_{\rm C}$ and $\rho_{\rm mag}(T) \approx const.$ for $T > T_{\rm C}$ (large)

Kubo-Greenwood:

$$\sigma(E) \propto {\rm Tr}[\delta(E-H)\mathbf{J}\delta(E-H)\mathbf{J}]\,, \quad \mathbf{J} = -i[\mathbf{R}, H]$$

where $\mathbf{J}$ is current operator and $\mathbf{R}$ are discrete coordinates of atomic sites
Turek et al. Phys. Rev. **65** 125101 (2002)
spin disorder resistivity: via disordered local moment (DLM) approach

SPIN DISORDER RESISTIVITY 1

at ambient pressure:

$$\rho(T) = \rho_0 + \rho_{\mathrm{vib}}(T) + \rho_{\mathrm{mag}}(T)$$

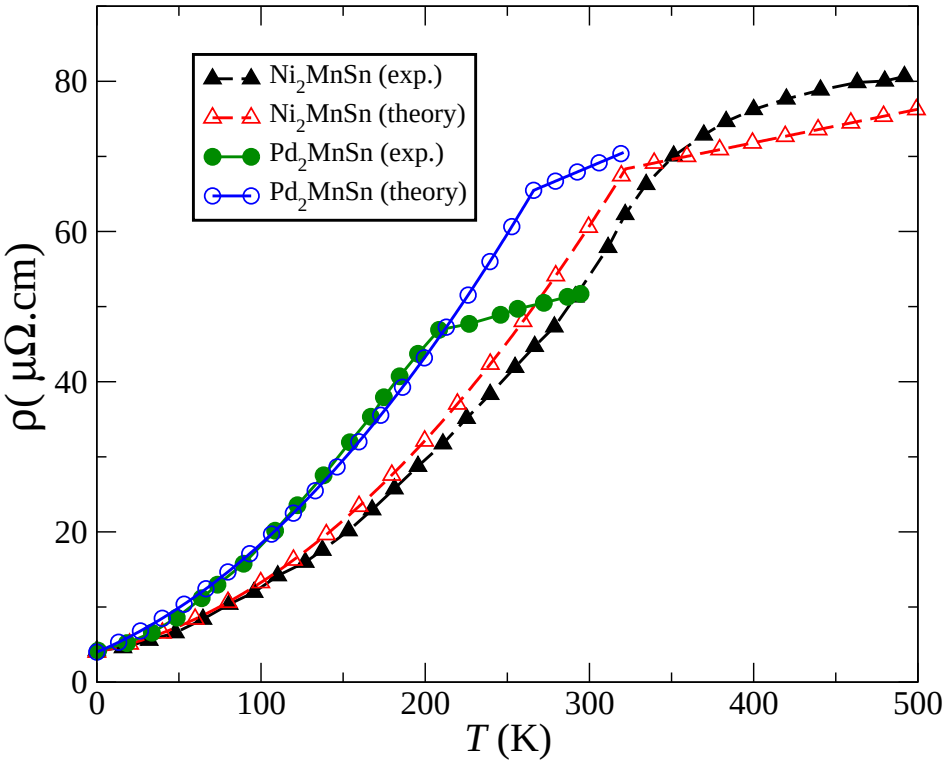
$$\rho_{\mathrm{vib}}(T) = aT$$

$$\rho_{\mathrm{mag}}(T) = \begin{cases} cT^2 & : \quad T < T_{\mathrm{C}} \\ \rho_{\mathrm{mag}}(T_{\mathrm{C}}) & : \quad T > T_{\mathrm{C}} \end{cases}$$

ρ_0, a from experiment

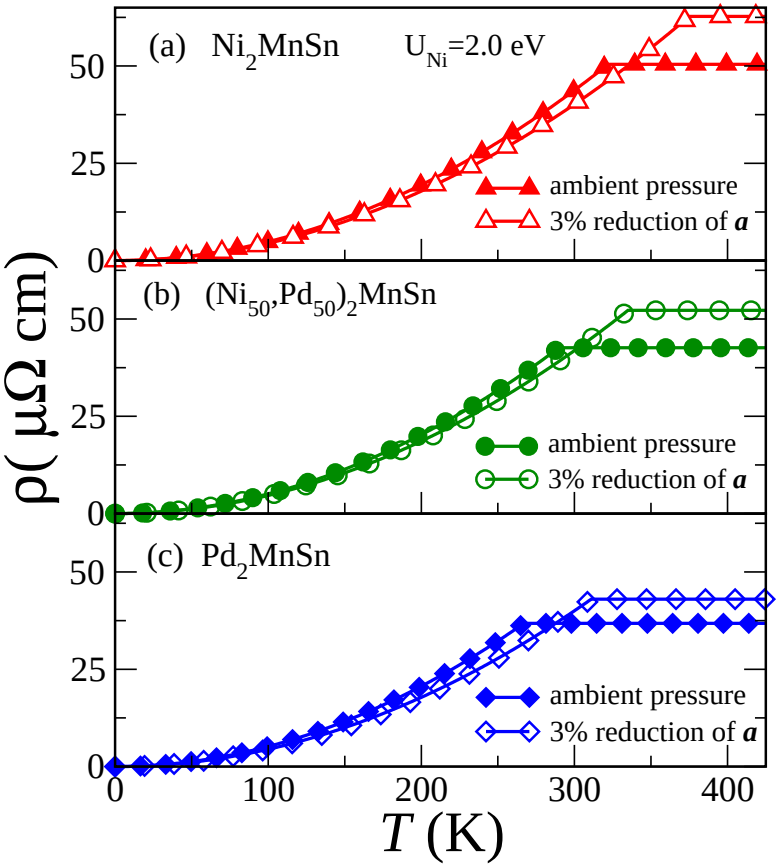
c from ab initio

$$c = \frac{\rho_{\mathrm{mag}}(T_{\mathrm{C}}^2)}{T_{\mathrm{C}}^2}$$



SPIN DISORDER RESISTIVITY 2

disorder at E_{F} is weak



two effects of pressure:

- band broadening and delocalization of states leads to a smaller ρ
- increase of T_{C} causes increased $\rho(T)$ for $T_{\mathrm{C}}(0) < T < T_{\mathrm{C}}(P)$

mostly theoretical predictions, experiment so far missing
experimental data are available only for a related compound Pd_2MnSb: increase of resistivity above T_{C} (Austin, Mishra 1967)

CONCLUSIONS

- T_{C} in $(\mathrm{Ni}_x\mathrm{Pd}_{1-x})_2\mathrm{MnSn}$ increases with pressure
- there are two regimes in $(\mathrm{Ni}_x\mathrm{Cu}_{1-x})_2\mathrm{MnSn}$:
  - T_{C} increases with pressure for $x < 0.7$
  - T_{C} decreases with pressure for $x > 0.7$
- explanation in terms of Anderson superexchange and Stearns indirect $d - d$ exchange
- pressure dependence of spin-disorder resistivity $\rho(T)$
  - $\rho(T)$ decreases for $T < T_{\mathrm{C}}(0)$
  - $\rho(T)$ increases for $T > T_{\mathrm{C}}(0)$