Can parity non-conserving weak interaction affects the crystal enantiomerically (chirality)?

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PROBLEM

Parity conserving electromagnetic interaction determines structure of any molecule or crystal.

Hence two different enantiomers (entities which are mirror images of each other) have to exist with equal probability.

I shall discuss an apparent violations of this rule and try to explain them using weak parity non-conserving interaction.

I do not consider here biological world. Apparently its chirality is a result of evolution and in remote worlds live can have different chiralities.

Experimental motivation

Non-centrosymmetric cubic crystals MnSi. It is very popular system due to helical magnetic structure, quantum phase transition to non-magnetic state at pressure etc.

There are four Mn and Si ions in the unit cell which can form two enantiomers: right and left.

Right.:Anticlochwise 120° rotation around (111).

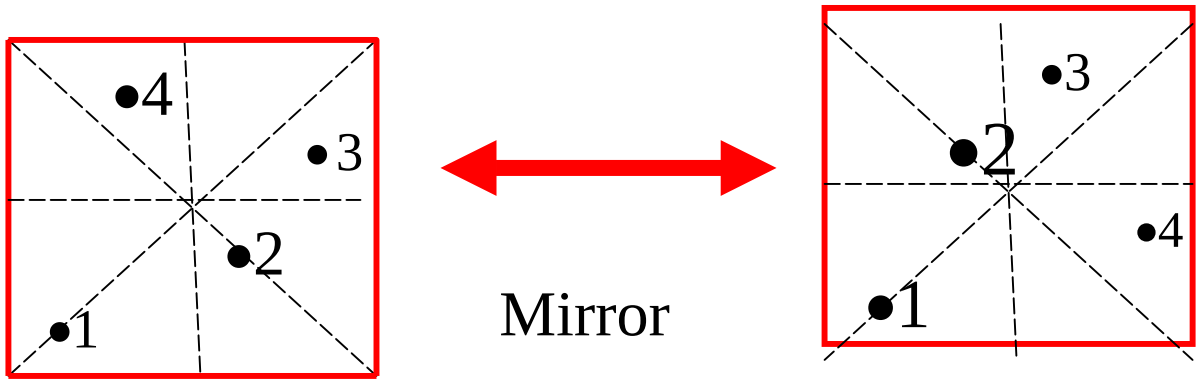
$$\mathbf{R}_1 = (u, u, u);$$
$$\mathbf{R}_2 = (1/2 + u, 1/2 - u, 1 - u);$$
$$\mathbf{R}_3 = (1 - u, 1/2 + u, 1/2 - u);$$
$$\mathbf{R}_4 = (1/2 - u, 1 - u, 1/2 + u).$$

Left: Clockwise 120° rotation around (111)

$$\mathbf{R}_1 = (u, u, u);$$
$$\mathbf{R}_2 = (1/2 - u, 1/2 + u, 1 - u);$$
$$\mathbf{R}_3 = (1/2 + u, 1 - u, 1/2 - u);$$
$$\mathbf{R}_4 = (1 - u, 1/2 - u, 1/2 + u).$$

$$u_{Mn} = 0.138; u_{Si} = 0.846; u_{Mn} + u_{Si} \approx 1.$$

Both structures are enantiomers: they are connected by mirror reflection in the plane perpendicular to (1,-1,0) direction.



R.H. L.H.

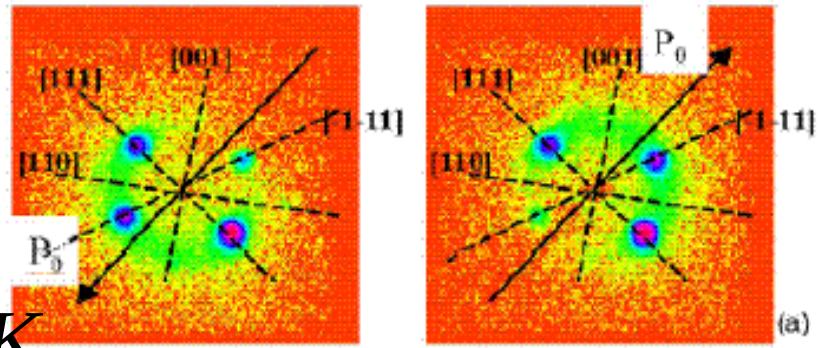
Unit cell projection on basal plane. Mn ions are shown.

First measurement (m.Tanaka et al.1985): Seven samples; All were left-handed! Since that the right-hand structure was not observed.

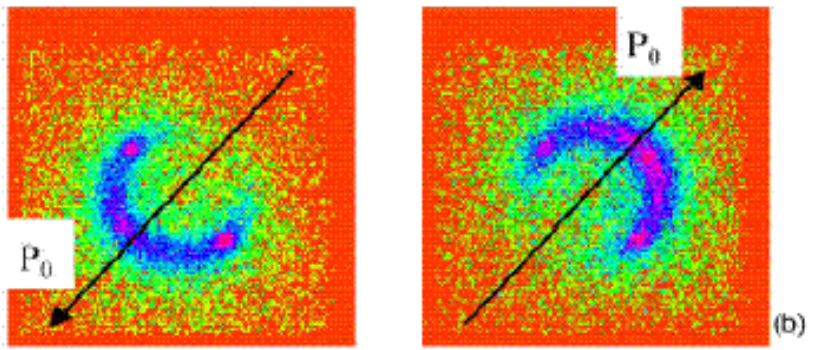
Recently the handness of the isostructure compound $Fe_{1-x}Co_xSi$ as function of doping x was studied (S.V.Grigoriev, D.Chernyshov et al.2008) was studied.

Left-right transition was observed at $x \approx 0.2$ along with strong changes of u_{Fe-Co} and u_{Si}. The left-handness of MnSi was confirmed also.

$T_C - 0.1K$



$MnSi; T_c\ 29K.$



$T_C + 0.2K$

Polarized neutron scattering (S.V. Grigoriev et al)

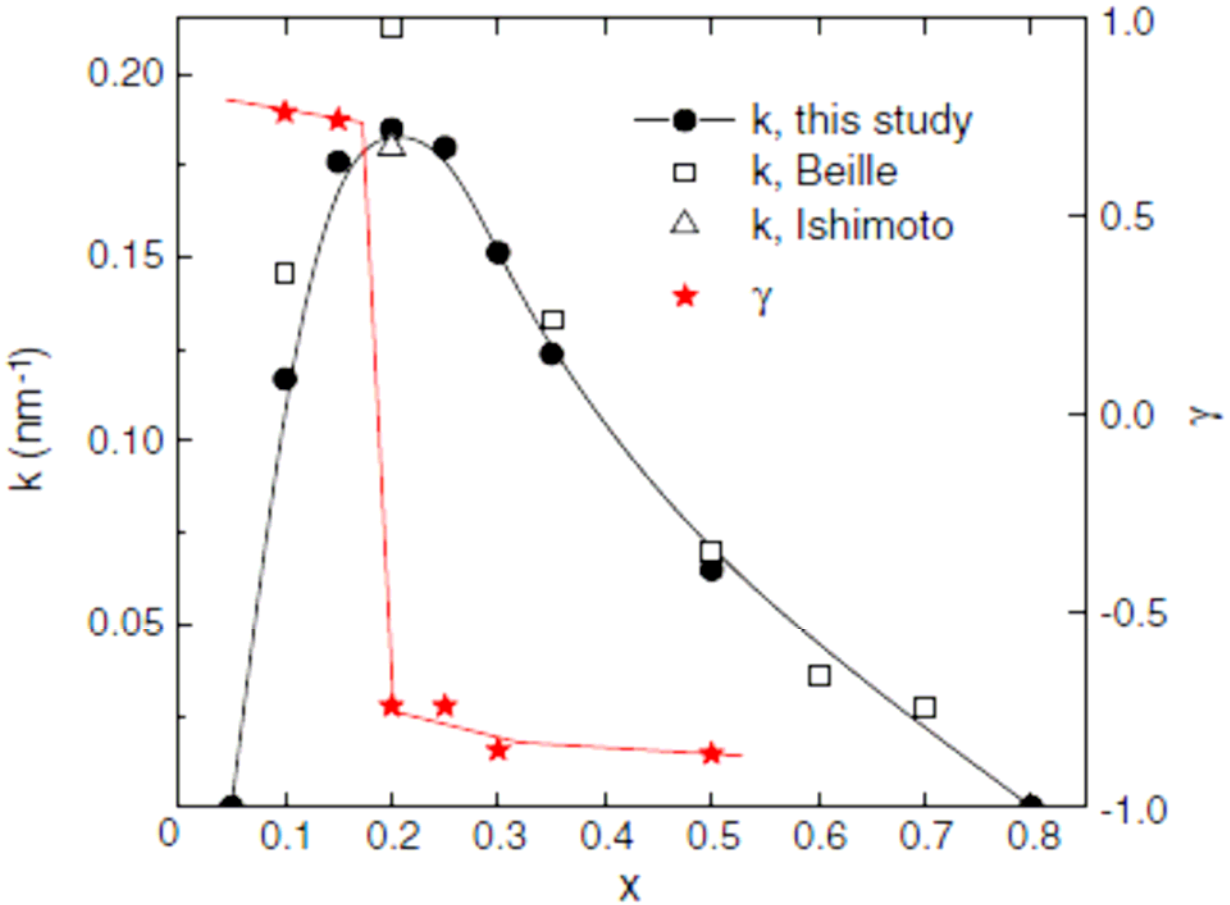
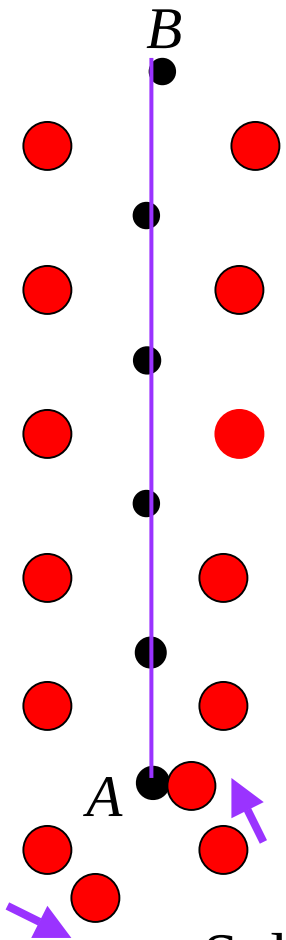


FIG. 3 (color online). Dependence of the helix wave vector k and the chirality γ on the Co concentration x for $Fe_{1-x}Co_xSi$ (□ [5], △ [6], ● this study).

S.V.Grigoriev,
D.Chernyshov et al.

$CsCuCl_3$ CHIRALITY



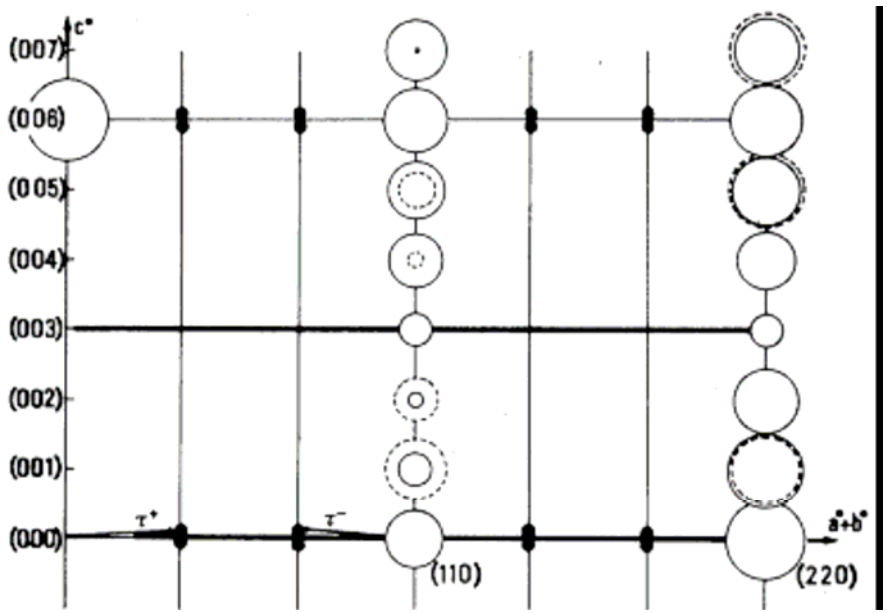
Jahn-Teller first order transition at T=423K.

Plain Cu-Cl chains above transition.

At T<423K Cu pairs rotate on 60° degree around AB line.

$\bullet - Cu^{2+}$

$\bullet - Cl^-$



K.Adashi et all.(1980)

Solid circles are observed Bragg intensities (Logarithmic scale)

Dashed circles are calculated intensities for left-handed rotation.

NATURE selects anticlockwise rotation!

Recent confirmation: V.P.Plakhty et al. (under preparation).

How consider these experimental findings?

Two ways:

Wait extra 20-30 years hoping for discovery lacking enantiomers.

Attempt to find a physical explanation for observed anomalies.

The second possibility is considered below.

Principal condition: The energy has to have pseudoscalar E_P term which has different sign in left and right systems.

It appears as a result of parity non-conserving weak interaction

(O.L.Zhizhimov, I.B.Khriplovich, ZK1982).

There are two forms of this interaction named as charged and neutral currents.

The former is responsible for beta-decay $n \to p + e + \bar{\nu}$

The second gives rise very weak parity non-conserving electron-nucleon interaction responsible for some tiny effects in atomic spectroscopy.

We consider this interaction and demonstrate that it can be enhanced strongly near the first order phase transition.

In non-relativistic form the electron- nucleon weak interaction is given by

$$W = \frac{G\kappa}{2m_e\sqrt{2}}[(\sigma \cdot \mathbf{p})\delta(\mathbf{r}) + \delta(\mathbf{r})(\sigma \cdot \mathbf{p})]$$

where $G = 1.02 \cdot 10^{-5} / m_p^2$, $\kappa_n = -0.5$, $\kappa_p = 0.04$,

and electron momentun $\mathbf{p} = -i\nabla$. (I.B.Khriplovich)

For single atom this interaction connects s and p states.

We outline here the ZK derivation of energy.

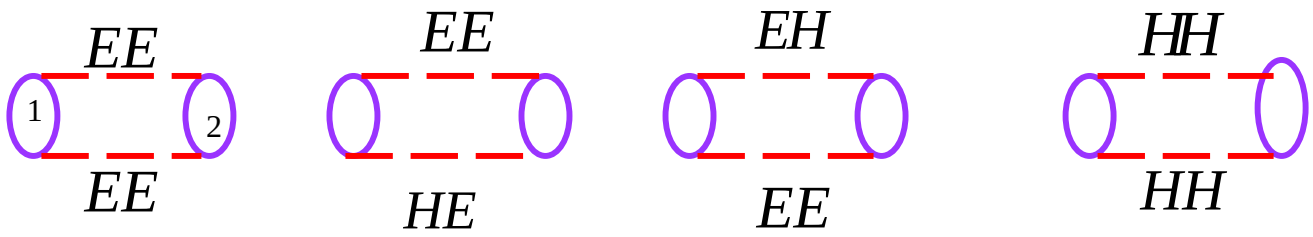
It is done by the same way as derivation of general van der Waals in the interaction.

Ions interaction with electromagnetic field is given by

$$V_{1,2} = -\mathbf{d}_{1,2}\mathbf{E}(\mathbf{r}_{1,2}) - \mu_{1,2}\mathbf{H}(r_{1,2})$$

Where $\mathbf{d}_{1,2}$ and $\mu_{1,2}$ are electric and magnetic dipolar momenta of two ions.

Interaction between two ions is represented by diagrams



where letters denote diagonal and off-diagonal electromagnetic field fluctuations.

The first diagram gives general expression for van der Waals interaction (see for example V.B. Berestetskii et al. Quantum Electrodynamics BLP).

The second two are not zero in the case of parity non-conservation (ZK interaction). They are a subject of this study.

The last one is neglected as very small.

General ZK expression for pseudoscalar energy at T=0 us given by

$$E_P = \frac{i}{4\pi}\int d\omega$$
$$[\alpha^{(1)}_{ik}(\omega) D^{EE}_{kl}(\mathbf{r}_{12},\omega)\beta^{(2)}_{lj}(\omega) D^{HE}(\mathbf{r}_{21},\omega) +$$
$$\tilde{\beta}^{(1)}_{ik}(\omega) D^{HE}_{kl}(\mathbf{r}_{12},\omega)\alpha^{(2)}_{lj}(\omega) D^{EE}_{ji}(\mathbf{r}_{21},\omega) +$$
$$(1 \leftrightarrows 2)]$$

$$\alpha_{ik}(\omega) = -\sum\left[\frac{<0|d_i|n><n|d_k|0>}{\omega-\epsilon_n+i\delta} - \frac{<0|d_k|n><n|d_i|0>}{\omega+\epsilon_n-i\delta}\right]$$

α is a conventional polarizability of an ion.

In non-magnetic case $\alpha_{ik} = \alpha_{ki}$.

$$\beta_{ik}(\omega) = -\sum\left[\frac{<0|d_i|m><m|\mu_k|0>}{\omega-\epsilon_m+i\delta} - \frac{<0|\mu_i|m><m|d_k|0>}{\omega+\epsilon_m-i\delta}\right]$$

β is parity non-conserving polarizability

In $\tilde{\beta}$ vectors $\vec{d}$ and $\vec{\mu}$ are interchanged. As $\vec{\mu}$ is t-odd we have $\beta_{ik}(\omega) = -\beta_{ki}(\omega)$.

Photon Green functions

$$D_{ij} = -i < TA_i(x_1)A_j(x_2) >; \quad D_{ij}(\omega, r_{12}) = -\left(\delta_{ij} + \frac{\nabla_i \nabla_j}{\omega^2}\right)\frac{e^{i|\omega|r_{12}}}{r_{12}}$$

As $\vec{E} = -\partial\vec{A}/\partial t$ and $\vec{H} = rot\vec{A}$, we have

$$D^{EE}_{ij}(\omega, r_{12}) = \omega^2 D_{ij}(\omega, r_{12}); \quad D^{HE}_{ij}(\omega, r_{12}) = -i\omega\epsilon_{inp}\nabla_n D_{pj}(\omega, r_{12})$$

and due t-oddness of magnetic field $D^{EH}_{ji}(\omega, r_{12}) = -D^{HE}_{ij}(\omega, r_{12})$

We are interested in small distances: r~lattice spacing. In this case (BLP, ZK)

$$E_P = -\frac{1}{2\pi r^5}\int d\omega\omega\left[\beta^{(1)}_{ik}\epsilon_{knl}\hat{r}^n_{12}\alpha^{(2)}_{lp}(\delta_{pi} - 3\hat{r}_p\hat{r}_i)\right.$$
$$\left.+\alpha^{(1)}_{ik}(\delta_{kl} - 3\hat{r}_k\hat{r}_l)\beta^{(2)}_{lp}\epsilon_{pni}\hat{r}^n_{21}\right]$$

If all tensors have the same structure $E_P \equiv 0$.

Pseudoscalar interaction may work if neighboring ions have different symmetry as in considered examples.

BETA POLARIZABILITY

Tensor $\alpha \sim [0.1nm]^3$ is conventional ion polarizability.
Al intermediate states "n" contribute to it formation.

Weak interaction connects "s" and "p" states only.

We are interested with Si and Cl ions with p external electrons and have to evaluate $\langle s|\mu_i|p\rangle$ and $\langle p|\mu_i|s\rangle$ matrix elements.

Without weak interaction they are zero and we have

$$\langle s|\mu_i|p\rangle = \langle \delta p|\mu_i|s\rangle + \langle p|\mu_i|\delta s\rangle$$

$$\delta|s>_\nu = \sum |p_\lambda> \sigma^\lambda_{\rho\nu} \frac{iG(Z\kappa_p + N\kappa_n)\Psi_s(0)\Phi(0)}{2m_e\sqrt{2}E_{sp}}$$

where λ enumerates orbital states of p electron: $\Psi^\lambda(\vec{r}) = r^\lambda \Phi(r)$,

ν and ρ are its initial and final spin states, Z and N are numbers of protons and neutrons in the nucleus.

In the case of Si and Cl ions the crystal field splits ground state p-electron orbits. They acquire index λ and we have

$$\beta_{ik}(\omega) = 2i(G/m_e)\mu_B\sqrt{2}(\kappa_n N + \kappa_p Z)\Psi_s(0)\Phi(0)$$

$$\sum \frac{\omega\delta_{i\lambda} < p_\lambda|d^\lambda|s > \delta_{\lambda k}}{E_{s\lambda}(\omega - E_{s\lambda} + i\delta)(\omega + E_{s\lambda} - i\delta)} \quad ; \mu_B > 0.$$

Final expression

$$E_P = -\frac{\Omega}{r^5}\sum_{\lambda_{12}}\Big[q^{(1)}_{ik}\epsilon_{knl}\hat{r}^n_{12}Q^{(2)}_{lp}(\delta_{pi}$$

$$-3\hat{r}_p\hat{r}_i) - Q^{(1)}_{ik}(\delta_{kl} - 3\hat{r}_k\hat{r}_l)q^{(2)}_{lp}\epsilon_{pni}\hat{r}^n_{12}\Big]$$

where $\Omega = \frac{2\sqrt{2}G\mu_B}{m_e}(\kappa_p Z + \kappa_n N)\Psi_s(0)\Phi(0)$ and two tensors

$$Q^{(1,2)}_{ik} = \sum \frac{\epsilon_n < 0|d^i|n >< n|d^k|0 >}{\epsilon_n + E_\lambda}; \; {}^{(1,2)}_{lj} = \sum \frac{\delta_{l\lambda} < p_\lambda|d^\lambda|0 > \delta_{\lambda j}}{E_\lambda}$$

In simplest case of two ions in different uniaxial surrounding

$$Q(q)_{ik}^{(1,2)} \rightarrow Q(q)\hat{z}_i^{(1,2)}\hat{z}_k^{(1,2)} \qquad (Q = \frac{3Q_{zz} - Q_{ll}}{2})$$

$$E_P = \frac{4\sqrt{2}G\mu_B}{m_e r^5} Qq(Z\kappa_p + N\kappa_n)\Psi_s(0)\Phi(0)$$

$$([\hat{z}_1 \times \hat{z}_2] \cdot \hat{r}_{12})[(\hat{z}_1 \cdot \hat{z}_2) - 3(\hat{z}_1 \cdot \hat{r}_{12})(\hat{z}_2 \cdot \hat{r}_{12})]$$

Numerical estimations

$$2\sqrt{2}Gm_e^2 = 8.5\times10^{-12}; \kappa_n = -0.5, \kappa_p = 0.04.$$

For mixing np and (n+1)s states $\Psi_s(0)\Phi(0) = \frac{Z^2}{[n(n+1)]^{3/2} a_B^4}$

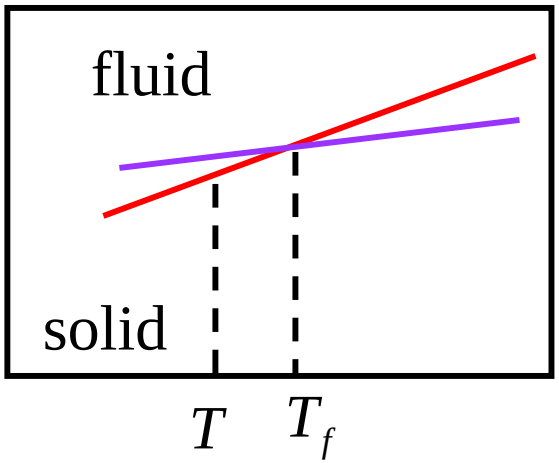
$2\mu_B Qq \sim \alpha^2 R_I^3 \nu / E_{eff}$ where R_I is the ion size and $\nu \sim 2 \div 3$

is effective number of p electrons.

From these expressions for Si-Si pairs in MnSi we obtain very rough estimation:

$$E_P \sim 10^{-13} \div 10^{-15} eV.$$

FIRST-ORDER TRANSITION AND THE WEAK INTERACTION ENHANCEMENT



The first order phase transition is a result of nucleation where new phase appears as bubbles which probability

$$w \sim e^{-E_B/T}$$

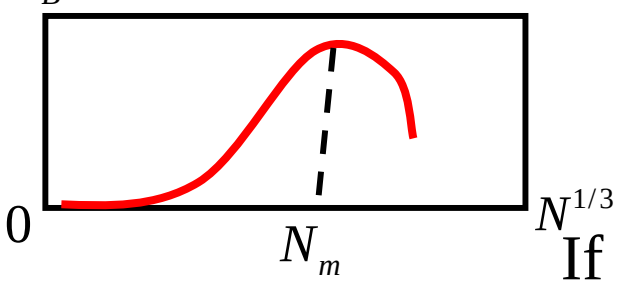
where E_B is a difference between the energies of a bubble and uniform liquid with same volume.

It is a sum of volume and surface energies and just below T_f is given by

$$E_B = 4\pi\varepsilon_c N(T - T_f)/3T_f + 4\pi a\varepsilon_c N^{2/3}$$

$0.1eV$ is an unit cell energy at low T, N is number cells in the bubble, a~1.

E_B This energy has maximum



$$E_m = \frac{\varepsilon_c}{3}\left[\frac{2aT_f}{T_f - T}\right]^2; \qquad N = N_m = \frac{2aT_f}{T_f - T}.$$

If $N < N_m$ the bubble is unstable and has to decay.

The growth begins when $N > N_m$.

But probability of the critical bubble is very small $W \sim \exp(-E_m/T)$

For sufficiently small difference $T_f - T$ product $\Delta = E_P N_m^3 z$

where z is nearest neighbor number may be comparable with $T_f \sim 0.1 eV$.

In this case for bubbles with different chiralities

$$W_{\pm} \sim exp\{-(E_m \pm \Delta)/T\}$$

and one enantiomer has to predominate.

From above estimations follows that it holds if $T_f - T \sim 10^{-4} T_f$.

For larger difference one has to get poly-crystal sample with randomly distributed single chiral grains.

It is a prediction which need experimental confirmation.

CHANGE OF CHIRALITY IN FeCoSi

In $Fe_{1-x}Co_xSi$ the left and right chirality was observed at x<0.2 and x>0.2 respectively (S.Grigoriev, D.Chernyshov et al.).

It was shown also that parameter u determining the Si position in the unit cell is equal to 0.157<1/4 at u=0.1 and 0.407>1/4 for u=0.25.

Value u=1/4 is a critical one: Each Si ion has two sets of the Si neighbors with distances

$$d_1 = \sqrt{1/4 + (1/2 - 2u)^2 + (1 - 2u)^2}; \qquad d_2 = \sqrt{1/4 + (1/2 - 2u)^2 + (2u)^2}$$

If u<1/4 we have $d_2 < d_1$; $d_1 < d_2$ for u>1/4.

So with growing u we have interchange the nearest neighbors.

Surprisingly pseudoscalar $P = ([\hat{z}_1 \times \hat{z}_2]\cdot\hat{r}_{12})[(\hat{z}_1\cdot\hat{z}_2) - 3(\hat{z}_1\cdot\hat{r}_{12})(\hat{z}_2\cdot\hat{r}_{12})]$

determining sign of E_P changed sign at u=1/4.

If the first-order enhancement works we have to have different chirality at u<1/4 and u>1/4.

CONCLUSIONS

Weak interaction may affect crystal enantiomericallity under following conditions:

- Neighboring ions have to have surroundings with different symmetry.
- Crystallization has to be very close to the freezing temperature T_f .
- Crystal field splitting of the ions levels has to be larger than T_f .