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# Electromagnetic Waves Generation in $Ni_{2.14}Mn_{0.81}GaFe_{0.05}$ Heusler Alloy at Structural Phase Transition

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Electromagnetic waves generated by the Heusler alloy $Ni_{2.14}Mn_{0.81}GaFe_{0.05}$ at structural phase transition was detected in the frequency range of 28–32 GHz. Influence of the kinetics of phase transitions on the nature of the sample millimeter radiation was studied as well. It has been observed that the contribution of the intrinsic radiation increases with increasing of the heating/cooling rate. The possible mechanisms and theory of such effect is discussed. It is shown that the maximum radiation intensity should be emitted in direction perpendicular to the movement of interphase boundary.

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## 1. Introduction

In recent years both theoreticians and experimentalists have heightened interest in new effects of electromagnetic waves generation under nonequilibrium processes in condensed media. Phase transitions (PT) of the 1st and the 2nd orders go at significant deviation from equilibrium state, and in this case the medium is active, i.e. is capable to emit energy as electromagnetic and/or acoustic waves. Therefore, there is a jump of magnetization $\Delta M$ or polarization $\Delta P$ of a sample at PT in the magnetic or electrodipole subsystem respectively, which lead to generation of electromagnetic and acoustic fields pulses [1, 2]. Structural PT of the 1st order has a more complex nature of the radiation. Structural PT goes during a certain time when nuclei of a new phase, phase boundaries, various defects, dislocations and fractures may form in the sample, that leads to the generation of electromagnetic and acoustic pulses [3]. The mechanisms of such effects may differ for different materials: ionic crystal, ice, metallic material, rock, etc. In metals, it may be the movement of electrons in the potential generated by the elastic strains around a dislocation. Near an edge dislocation of semiconductors the unfilled valence bonds play a role of acceptor sites, and so, have an effect on recombination processes and/or carrier mobility [4]. Plastic deformation may also lead to the emission of free electrons, ions, photons, etc. from the surface. Electromagnetic radiation emission in metallic materials due to plastic deformation, plastic flow, crack initiation and propagation, and fracture has been well investigated [5–7]. Nevertheless, electromagnetic waves emission during PT in materials is yet to be explored deeper.

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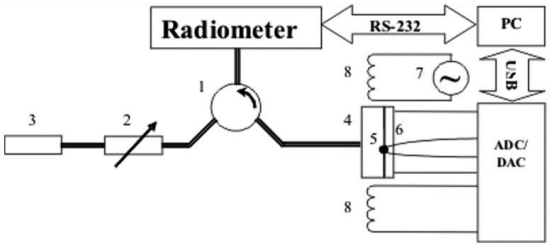


Fig. 1. The diagram of experimental setup: 1 — the circulator, 2 — the attenuator, 3 — the load is cooled by liquid nitrogen, 4 — the sample, 5 — the thermocouple, 6 — the Peltier element, 7 — the generator (17 kHz), 8 — the two-coil magnetometer.

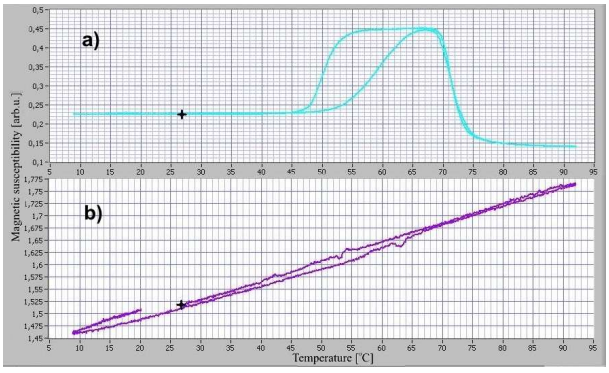


Fig. 2. The temperature dependences of (a) the magnetic susceptibility, (b) the radiation intensity of the sample when it was heated up to 92 °C and was cooled after that. The heating/cooling rate was 1 K/s.

The 2nd order paramagnetic-ferromagnetic PT ($T_c$ = 75 °C) and the magneto-structural of 1st order austenite-martensite PT ($T_m$ = 45–65 °C) occur in the Heusler alloy $Ni_{2.14}Mn_{0.81}GaFe_{0.05}$, see Fig. 2a [8, 9]. In this work we observe experimentally the electromagnetic wave emission from the free surface

of the $Ni_{2.14}Mn_{0.81}GaFe_{0.05}$ sample at the magneto-structural PT. We also discuss a possible mechanisms and theory of such effect.

## 2. Experiment

The ability to self-radiation of electromagnetic waves from the free surface of the sample Heusler alloy $Ni_{2.14}Mn_{0.81}GaFe_{0.05}$ has been experimentally investigated in the wavelength range of 8 mm. For the investigation of the sample radiation and to separate the contributions from radiation caused by the PT, and the contribution from the changes in the reflection coefficient of thermal radiation environment in the frequency-domain of 28–32 GHz, an original experimental setup has been developed (Fig. 1). It includes a Heusler alloy test sample as a plate with dimensions $10 \times 10 \times 0.5$ mm with a temperature control system in the range from 0 to +100 °C, magnetometer for registering the magnetic susceptibility of the sample *in situ*, heterodyne type radiometer (bandwidth 28–32 GHz) with the waveguide in direct contact with the sample, circulator, radiating load whose temperature can vary from room temperature to liquid nitrogen by attenuator. Miniature thermocouple was installed directly on the sample surface.

Analysis of the typical dependences of the radiometer signal (Fig. 2) shows that the radiation of the sample is a nonmonotonic function of temperature, and near the magneto-structural PT it has evident anomalies (at 53–55 °C and 62–64 °C), see Fig. 2b). The peaks of the radiation do not disappear when the temperature of the load increases from the nitrogen to the room temperature, Fig. 3. The nonmonotonic anomalies are visible very well. It proves that the external radiation reflected from the sample surface with different coefficients in different structural phases does not explain the registered radiometer peaks. Influence of the kinetics of PTs [10] on the nature of the sample millimeter radiation has been studied with the change in heating/cooling rate from 0.1 K/s to 10 K/s. It has been observed that the contribution of the intrinsic radiation increases with increase in the heating/cooling rate. It also confirms that the detected anomalies are associated with the intrinsic radiation of electromagnetic waves from the sample at the magneto-structural PT.

## 3. Possible mechanisms and theory

The structural PT occurs during a certain time. During this time embryos of new phase interphase boundary, multiple defects, dislocations and cracks can be formed in the sample, which also leads to the generation of electromagnetic pulses. All these defects are accompanied by the formation of inhomogeneous elastic deformations. At the structural PT existence of inhomogeneous deformation (for example, on the interphase boundary) leads to redistribution of the electron density near the defect $\Delta n(z)$. We will follow the works [11, 12] for calculation of this redistribution. Let us consider a model function of mechanical stress $\sigma_{\mathrm{M}}(z)$:

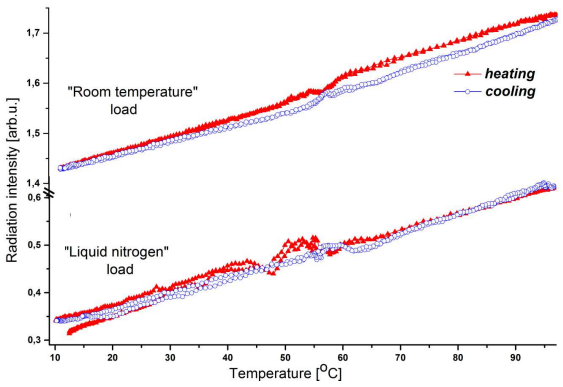


Fig. 3. Temperature dependence of the radiation intensity of the sample at different positions of the attenuator. The heating/cooling rate was 2 K/s.

$$\sigma_{\mathrm{M}}(z) = \begin{cases} 0, & -\infty < z < 0, \\ \sigma_0 z/d, & 0 \le z < d, \\ \sigma_0, & d \le z < \infty. \end{cases} \tag{1}$$

Here, $\sigma$ is a parameter characterizing change in mechanical stress from one area to another, $d$ is an effective length where change of $\sigma_{\mathrm{M}}(z)$ occurs. Such a function of mechanical stress describes transition between the regions of the material with different stress by the simplest way. Within the framework of model in which the state of the conduction electrons of an alloy is described by a single orbital nondegenerate band the strain created by mechanical stress can cause a band shift in energy. The Hamiltonian that includes such an effect has a form [11, 12]:

$$H = \sum\nolimits_{i\sigma} \left[\omega + SU\left(\boldsymbol{r_i}\right)\right] c^{+}_{i\sigma} c_{i\sigma} + \sum\nolimits'_{ij} \sum\nolimits_{\sigma} \lambda^{0}_{ij} c^{+}_{i\sigma} c_{j\sigma} + 0.5 \sum\nolimits_{i} K_A \Omega_0 U^2\left(\boldsymbol{r_i}\right) + H_{\mathrm{Coul}}. \tag{2}$$

Here, $c^{+}_{i\sigma}$ ($c_{i\sigma}$) is the Fermi creation (annihilation) operator of an electron with spin $\sigma$ in a localized Wannier state $i$; $\omega$ is the energy that characterizes the position of the center of the electron band; $\lambda^{0}_{ij}$ is the electron-mixing integral in an undeformed lattice; parameter $S$ describes the shift of the conduction band during strain; $K_A$ is the elastic stiffness of the lattice, $\Omega_0$ is the initial volume of the unit cell; $H_{\mathrm{Coul}}$ is the Hamiltonian of the Coulomb electron–electron interaction.

To determine the strain parameter $U(\boldsymbol{r})$ one has to use the condition of mechanical equilibrium $\langle \partial H/\partial U\left(\boldsymbol{r}\right)\rangle = \sigma_{\mathrm{M}}(z)V$, where $V$ is the volume of the crystal. The concentration of conduction electrons $n(\boldsymbol{r})$ may be defined in the form $n\left(\boldsymbol{r}\right) = \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \left\langle c^{+}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}'\sigma}\right\rangle \mathrm{e}^{-\mathrm{i}\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}$.

In general, the problem reduces to solving a system of five equations: for the concentration of conduction electrons, the electrostatic potential (the Poisson equation) that results from the electron-density change $\Delta n(z) = n(z) - n_{0\mathrm{es}}$ ($n_{0\mathrm{es}}$ is the mean concentration of electrons arriving at a lattice point, taking into account the electron–strain interaction), the wave function of an electron in the neighborhood of a defect, the Green function, and

the chemical potential. Solving this system of equations one can get electron-density change for mechanical stress $\sigma_{\rm M}(z)$ (1) [12]:

$$\Delta n(z)=$$

$$\begin{cases} eR_sD\left(2\lambda_{1s}\right)^{-1}\left(1-\mathrm{e}^{-\lambda_{1s}d}\right)\mathrm{e}^{\lambda_{1s}z}, & -\infty < z < 0, \\ eR_sD\left(2\lambda_{1s}\right)^{-1}\left(\mathrm{e}^{-\lambda_{1s}z}-\mathrm{e}^{\lambda_{1s}(z-d)}\right), & 0 \le z < d, \\ -eR_sD\left(2\lambda_{1s}\right)^{-1}\left(1-\mathrm{e}^{-\lambda_{1s}d}\right)\mathrm{e}^{-\lambda_{1s}(z-d)}, & d \le z < \infty. \end{cases} \quad (3)$$

In (3) $e$ is the electron charge, $\lambda_{1s} = (eR_s/\varepsilon_0)^{1/2}$, $D = SU_0/ed$,

$$R_s = \left(\frac{3n_0}{8\pi^4}\right)^{1/3} \times \frac{\left[1+S^2 n_0^{1/3}/\left(3\pi^2\right)^{2/3}\alpha K_A\right]^{1/2}}{\alpha\left\{1-\left(\frac{3n_0}{8\pi^4}\right)^{1/3}\frac{S^2}{\alpha K_A}\left[1+\frac{S^2 n_0^{1/3}}{(3\pi^2)^{2/3}\alpha K_A}\right]^{1/2}\right\}},$$

$n_0$ is the mean concentration of electrons, without taking into account the electron–strain interaction; $\alpha = \hbar^2/2m^*$, $m^*$ is an effective mass of the electrons. $n_{0\rm es}$ and $n_0$ are connected by the equation $n_{0\rm es} = n_0\left[1+S^2\sqrt[3]{n_{0\rm es}}/\sqrt[3]{9\pi^4}\alpha K_A\right]^{3/2}$.

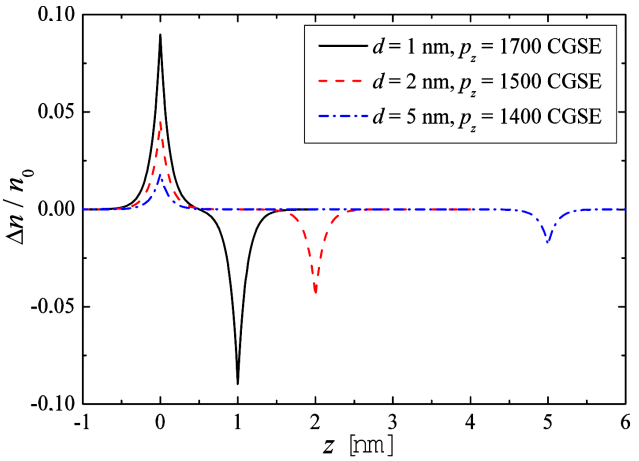


Fig. 4. Relative electron-density change for different effective lengths of the interphase boundary $d$. In inset there are presented values of equivalent electro-dipole moments $p_z$ for unit square of the interphase boundary.

In Fig. 4 there are shown results of calculation of electron-density change (3) for different effective length $d$ where change of $\sigma_{\rm M}(z)$ occurs with the typical values of parameters: $S = 4$ eV, $U_0 = 0.1$, $n_0 = 16\times10^{-4}$ Å$^{-3}$, $K_A = 0.4$ eV/Å$^3$, $\alpha = 3.8$ eV Å$^2$. One can see that electron redistribution looks like an electric dipole. Increase of effective interphase boundary length leads to increase in dipole arm and to reducing of an effective charge. One can to calculate an electric dipole moment of such redistribution: $p_z = -eS_0\int z\Delta n(z)\,\mathrm{d}z$, where $S_0$ is the interphase boundary square.

The calculations show that effective electric dipole moment almost does not depend on the interphase boundary length (at least by order of magnitude). Its increase leads to very slow decrease in electric dipole moment.

The movement of interphase boundary may be represented as moving dipole $P_z(z,t) = p_z\delta(z-vt)$. Such moving dipole is a source of electromagnetic waves radiation.

Solution of the moving dipole radiation problem is well known. The intensity of radiation at frequency $\omega$ in the direction defined by angle $\theta$ with $z$-axis, along which moves the dislocation has the form: $I_{\theta\omega} = \omega^4 8^{-1}\pi^{-2}c^{-3}p_z^2\sin^2\theta$. Here, $c$ is the speed of light in vacuum. One can see that the maximum radiation intensity will be emitting in direction perpendicular to the moving one. We made some estimates of the maximum intensity: for frequency $\omega = 10^{10}$ rad/s and $S \approx 20$ nm$^2$, $I_{\omega\,\max} \approx 1.4\times10^{-2}$ erg/(s cm$^2$) if $d = 1$ nm, $I_{\omega\,\max} \approx 1\times10^{-2}$ erg/(s cm$^2$) if $d = 2$ nm, and $I_{\omega\,\max} \approx 9\times10^{-3}$ erg/(s cm$^2$) if $d = 5$ nm. In real materials electromagnetic energy will mainly emit from the surface of the sample due to its skin effect.

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