Anomalies in the elastic properties of heavy rare-earth metals in the region of the phase transition to the magnetically ordered state

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Based on the theory of second-order phase transitions, a model describing anomalies of elastic constants near the transition to a magnetically ordered state for a hexagonal helical antiferromagnet has been developed. The theoretical model has been confirmed by experimental measurements of Young's modulus in a terbium single crystal. [S0163-1829(97)09321-1]

Heavy rare-earth metals (REM's) are characterized by complex magnetic-spin structures and phase transitions,[1-3] which leads to different anomalies in their elastic properties. Negative discontinuities in elastic stiffness c_{ii} ($i=1,2,3$) and Young's modulus E along the crystallographic axes a, b, and c were experimentally observed[1,3] at the temperature where the transition from a paramagnetic to magnetically ordered state in heavy REM's occurs. In spite of the considerable amount of existing experimental studies with regard to elastic properties of heavy REM's the nature of anomalies at the magnetic phase transition points is still not quite clear.[3,4]

Available up-to-date experimental results on the elastic properties of terbium are discussed in Refs. 1 and 4. Negative anomalies of Young's modulus observed in heavy REM's during the transition to a magnetically ordered state were assumed[5-7] to be due to additional magnetostrictive deformations of the sample caused by the changes in spontaneous magnetization under the influence of mechanical stress on the sample during the measurements (so-called "mechanostriction of paraprocess"). The thermodynamic theory of the second-order phase transitions considering relaxation processes in a single-domain isotropic ferromagnet was used in Refs. 5 and 6 for the description of the Young's modulus anomaly at the Curie temperature. In this simplest case the magnetoelastic energy can be written as a power series of mechanical stress p:

$$W_{me} = -(\gamma p \sigma^2 + \varepsilon p^2 \sigma^2 + \cdots), \tag{1}$$

where γ and ε are the magnetoelastic coupling parameters and σ the specific magnetization. The second term in Eq. (1), which is proportional to the square of the spontaneous magnetization σ_s^2, was taken into account in Ref. 6, and the Young's modulus anomaly due to this term was associated with the change of bonding forces between the atoms in a crystalline lattice arising from the magnetostrictive deformations in the magnetically ordered state. The elastic compliance anomalies at the Néel temperature Θ_N for hexagonal helical antiferromagnets were studied in Ref. 7; however, the magnetoelastic energy expansion was restricted to terms linear with respect to the mechanical stress. In our paper the problem is solved in a more general form considering the products between the magnetization vector components and the squared combinations of the mechanical stress tensor components in the magnetoelastic energy.

Consider a single-domain antiferromagnet with helical spin structure below the magnetic ordering temperature Θ_N which belongs to the Laue class $6mm$ (D_{6h}^4). The magnetic moments in such a spin structure are placed in the basal planes which are perpendicular to the hexagonal axis c. The magnetic moments of atoms in these basal planes are ferromagnetically ordered with the angle φ between the moments in the neighboring layers (helical turning angle). The total energy of such an antiferromagnet can be written in the form

$$W = W_e + W_h + W_{ex} + W_{me} - H_i \sigma_i, \tag{2}$$

where W_e is the elastic energy, W_h is the energy of spin structure, W_{ex} is the exchange energy in the basal plane, W_{me} is the magnetoelastic energy, and H is the magnetic field. According to Ref. 8, W_e is defined by the equation

$$W_e = -[S_{11}(T_1^2 + T_2^2)/2 + S_{12}T_1T_2 + S_{13}(T_1 + T_2)T_3 + S_{33}T_3^2/2 + S_{44}(T_4^2 + T_5^2)/2 + (S_{11} - S_{12})T_6^2], \tag{3}$$

where T_i and S_{ij} are the components of the elastic stresses and elastic compliance tensors. The two interchangeable indices in Eq. (3) are replaced by a single index according to the scheme $11=1$, $22=2$, $33=3$, $12=21=6$, $13=31=5$, $23=32=4$. The energy of the helical spin structure can be expressed using the model proposed in Ref. 9 as follows:

$$W_h = -\sigma^2(n_1 \cos\varphi + n_2 \cos 2\varphi), \tag{4}$$

where n_1 and n_2 are the exchange parameters for the nearest- and next-to-nearest-neighboring basal planes ($n_1 > 0$ and $n_2 < 0$). The parameters n_1 and n_2 are assumed to have a linear dependence on the interplanar spacing:

$$n_i = n_{i0} + (\partial n_i / \partial \ln c)\epsilon_c, \tag{5}$$

where ϵ_c is the c-axis strain.

It is assumed that magnetic moments are completely within the basal plane and that the basal plane exchange energy W_{ex} can be expressed near the magnetic ordering temperature as follows:

$$W_{ex} = (\alpha/2)\,\sigma^2 + (\beta/4)\sigma^4 + \cdots, \tag{6}$$

where α and β are the thermodynamic coefficients.

In our paper the orthogonal axes x, y, and z correspond to the crystallographic axes a, b, and c, respectively. Let us

