GENERALIZED CONTINUAL THEORY OF DISLOCATIONS

Y.M. KRITCHEVETS, I.M. TITARENKO and A.A. KARTYSH

Institute of the Theoretical Material Research,
Naukova Str., 3b, Lviv, 290601, Ukraine

ABSTRACT

The generalization of the continual theory of dislocations is made by the application of differential geometry and topology methods,namely the theory of fiber-bundles. In such an approach the disordered system is described as the fibre-bundle P(M,G) with base $M = R^4 \oplus V^{\infty}$ and structural group G = U(1). In order to account the influence of electron system this construction is supplemented by the associated fiber-bundle E(M,G,H,P), where H - is the standard layer (space of the Hilbert space). Components of the distortion vector correspond to the connectivity coefficients, while components of the dislocations flux density tensor correspond to the curvature tensor of the main fiber-bunle.

KEY WORDS

Continual theory of dislocations, fiber - bundle,connectivity coefficients,curvature tensor,structural group,distortion vector, dislocations flux density tensor, quantum equation of motion,account of electron system influence.

A considerable number of models that describe mechanical properties of defect crystalls have been developed lately. For the analysis of defect influence on optical,electrical and mechanical properties models which take into account the influence of the degree of ordering of crystalls on their electron substructure are required.

Thus,one can try to find a connection between the continual theory of dislocations and the quantum equation of motion on the base of which physical characteristics of crystall can be evaluated.The goal of this paper is to obtain the quantum equation of motion which includes information about disordering of crystall described in terms of continual theory of dislocations. By its very nature continual theory of dislocations is a geo-

metrical model. Therefore it is natural to use methods of differential geometry, specifically certain representations of the theory of fiber-bundle for its generalization (Konoplyova,Popov 1980;. Jeicher, 1981). Describing the defect crystall with the help of fiber-bundle we can choose the space $R^4 \otimes V^{\infty}$ as a basis and certain Lee group as a fibre (Gelobenko,Shtern, 1983; Adams, 1978).The influence of the electron subsystem is taken into consideration by the supplementation of this construction by an associated fibre-bundle where the standard layer H is chosen to be a separable subspace of the Hilbert space.Diagram,that corresponds to the construction has the form:

$$\begin{array}{ccc} P(M,G) & \longrightarrow & E(M,G,H,P) \\ {\scriptstyle \pi_1}\downarrow & & \uparrow{\scriptstyle \pi_2} \\ M & \longleftarrow & \end{array} \qquad (1)$$

where: M - is a basis;
P(M,G)-is the main fiber-bundle with the structural group G;
E-is an associated fiber-bundle with the standard layer H;
π_1,π_2-are the corresponding projections.

For structural droup G choosing we can use the description of the continual theory of dislocations made by Dzyaloshinskii (1981),where the main equations are written in the form:

$$J^{a}_{\alpha\gamma} = \partial_{[\alpha}\beta^{a}_{\gamma]} \qquad (2)$$

Here: $J^{a}_{\alpha\gamma}$ - is the dislocations flux density tensor;

β^{a}_{α} - is a distortion 4-vector.

Equations system (2) is invariant to gauge transformations:

$$\beta^{a}_{\alpha} \longrightarrow \beta^{a}_{\alpha} + \partial_{\alpha}\lambda \qquad (3)$$

(2) and (3) relations analysis shows that gauge potentials correspond to the connectivity coefficients of the main fibre bundle with the structural group U(1).In the present case the equation for the curvature tensor of the fiber-bundle

$$R^{a}_{\mu\nu} = \partial_{[\mu}\Gamma^{a}_{\nu]} - \frac{i}{2} f^{a}_{bc}\,\Gamma^{b}_{[\mu}\,\Gamma^{c}_{\nu]} \qquad (4)$$

where: $R^{a}_{\mu\nu}$ - is a curvature tensor;

Γ^{a}_{ν}- are the connectivity coefficients;

f^{a}_{bc} - are the connectivity constants of the group,reduces to the expression:

$$R^{a}_{\mu\nu} = \partial_{[\mu}\Gamma^{a}_{\nu]} \qquad (5)$$

Here and further greek indeces refer to the base, while latin

indeces refer to the layer. Analysis of equations (2) and (5) indicates that the dislocations flux density tensor corresponds to the curvature tensor of the space P(M,G). For the account of the electron subsystem associated fibre-bundle with the standard fibre chosen as the Hilbert space of bispinors H is being built.Physical sense of their gauge transformations:

$$\Psi \longrightarrow \Psi e^{i\alpha} \qquad (6)$$

consists in the phase invariance of observed values.Diagram, that corresponds to the construction has the form:

$$\begin{array}{ccc} P(M,U(1)) & \longrightarrow & E(M,U(1),H,P) \\ {\scriptstyle \pi_1}\downarrow & & \uparrow{\scriptstyle \pi_2} \\ M & \longleftarrow & \end{array} \qquad (7)$$

where E- is an associated fiber-bundle;π_2:E $\longrightarrow$ M.

Then the simplest Lagrange function that includes the electron subsystem can be defined as:

$$L = L_o + L_1 \qquad (8)$$

where:

$$L_o = J^{a}_{\mu\nu}\,J^{\mu\nu}_{a} \qquad (9)$$

$$L = \bar{\psi}\,\gamma^{\mu}\,\partial_{\mu}\psi - \partial_{\mu}\bar{\psi}\,\gamma^{\mu}\,\psi - \frac{i}{2}\left(\bar{\psi}\,\gamma^{\mu}\,I_a\,\beta^{a}_{\mu}\,\psi + \bar{\psi}\,I_a\,\beta^{a}_{\mu}\,\gamma^{\mu}\,\psi\right) - m\,\bar{\psi}\,\psi \qquad (10)$$

Here: ψ - are the bispinors;

γ^{μ}- are Dirak matrices;

I_a - is the structural group generator;

m - is the carrier mass.

After the standard variation procedure we obtain the equation for the distortion tensor:

$$\partial_{\nu}\partial_{[\mu}\beta^{a}_{\nu]} = \frac{i}{2}\left(\bar{\psi}\,\gamma^{\mu}\,I_a\,1^{a}_{\mu}\,\psi + \psi\,1^{a}_{\mu}\,I_a\,\gamma^{\mu}\,\bar{\psi}\right),^{a}_{\mu} \qquad (11)$$

where 1^{a}_{μ} -is the unit matrix.

The equation (11) describes change of the dislocations flux density tensor in consequence of the electron subsystem influence and therefore we can regard it as the generalization of the continual theory of dislocations.The motion equation can be obtained by variation of Lagrange function on bispinors. This

equation has a following view:

$$(i\gamma^{\mu}\partial_{\mu} \frac{i}{2}\gamma^{\mu} \underset{\alpha}{I} \beta^{\alpha}_{\mu} - m)\ \psi = 0 \qquad (12)$$

It enables to evaluate the influence of the structural disordering degree of crystall on its properties.Its nonrelativistic limit has the form:

$$i\frac{\partial\psi}{\partial t} = \left[-\frac{1}{2m}\left(\nabla^2 - i\hat{\beta}\nabla + \hat{\beta}^2\right) + \beta_o - \frac{1}{2m}\sigma\hat{\alpha}\right]\psi \qquad (13)$$

where: $\hat{\beta}$ - is the reduced tensor of distortion;

$\hat{\alpha}$ - is the dislocations flux density 3-tensor;

β_o - is the time component of the distortion;

σ - are Pauli matrices.

The solution of the equation (13) for the case when distortion is modulated by the sum of the modified Vud-Saxon potentials.

$$\beta(y) = \frac{\alpha y^2 + 2y + \alpha}{\alpha y^2 + (1+\alpha^2)y + \alpha} \qquad (14)$$

where :$y = e^{-x/l}$, $\alpha = e^{-a/l}$

l - is the mean size of the transition from deformed to nondeformed area.

2a - is the size of the distorted area when $l \to 0$,

has a view:

$$\psi_{\pm} = C_1 \sum_{\nu} e^{ikx}\ \mu_{\nu}\ \exp\left(\mp\frac{x}{l}\nu\right) + C_2 \sum_{\nu} e^{-ikx}\ \mu_{\nu}\ \exp\left(\mp\frac{x}{l}\nu\right) \qquad (15)$$

where: k - is a quazi-momentum.

Coefficients can be determined from the reccurent relations:

$$\sum_{k=0}^{6}\mu_{\nu-k}\ \alpha_k(\nu-k)(\nu-k-1) + \sum_{k=0}^{5}\mu_{\nu-k}\ \beta_k(\nu-k) + \sum_{k=0}^{4}\mu_{\nu-k}\ \gamma_k = 0 \qquad (16)$$

In the regarded case of the localized distortion the solution of the motion equation is the plane wave with modulated amplitude.The character of the modulation is determined by the the distortion parameters.

In the limit of $l \to 0$ the relation(14) describes the unit distortion,localized near point X=0.In this case the relation (15) is considerably simplified.Only the terms with $\nu = 0$,which describe wave function change near unit distortion are left. The solution when $|X| \to \infty$ has a similar character.

Using (15) and (16) makes it possible to analiyze the influence of the electron system on the character of dislocations distribution and motion.

REFERENCES

J. Adams (1978) Lectures on Lee Groups. Nauka,Moscow.
J.Dzyaloshinskii (1981) Gauge Theories and Densities of Topological Singularities,Conf.on Defect Physics,Amsterdam.
D.P.Gelobenko,A.I.Shtern.(1983) Reprezentations of Lee Groups. Nauka,Moscow.
H.Jeicher (1981) Gauge Fields for Electrons in crystalls with topological defects.Phys.lett.V.87A,N3,p.113-115.
N.I.Konoplyova,V.N.Popov (1980) Gauge Fields.Atomizdat,Moscow.