Statistical methods in dislocation dynamics

Main results of the PhD thesis

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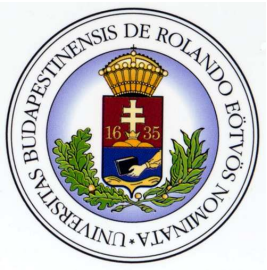

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Introduction

The plastic deformation of crystalline materials in most cases is caused by collective motion of dislocations. These line-like lattice defects interact with each other via the $1/r$ type, i.e., long-range, mechanical stress field generated by a single dislocation. In addition, their movement is constrained to a glide plane. As a result, these systems are strongly coupled and in many aspects peculiar. As an example we can mention the dislocation patterns that evolve in crystals or the dislocation avalanches. Since these phenomena are closely related to the plastic response of a crystalline material, their understanding is a key issue in materials science.

In practice, plastic deformation is usually described by phenomenological models, which usually construct constitutive laws between the stress, strain, strain rate and dislocation density. These models give satisfactory predictions under quite general conditions and at large specimen sizes. It turned out, however, that as soon as any characteristic length scale of the deformation or the material (such as the size of the indenter, the specimen size, grain size, size of precipitates, etc.) is in the order of 1 μm, the observed mechanical properties differ from the ones predicted by classical models. In the theory of plasticity this phenomenon is called size-effect.

With the fast development of nanotechnology, the small samples happened to become the subject of growing interest. In order to account for size-effects, nonlocal phenomenological models were worked out, which turned out to be successful in many aspects (they are able to account for small size hardening or for some kind of dislocation patterns). A major disadvantage of these models is that the fact that the basic mechanism of plastic deformation is dislocation motion is not included at all. Instead, parameters with length dimensions appear as the coefficients of gradient terms. The origin of these parameters is not clarified. Therefore, there are many such dislocation-related phenomena, that cannot be described by such models. It was found, for instance, that the plastic deformation of a single crystal pillar with diameter of 1 μm is substantially different from the macroscopic case. The deformation takes place intermittently in distinct areas. As a practical consequence, this avalanche-like behaviour precludes the predictable forming of thin wires.

In the last 15 years the behaviour of dislocation systems is more and more fre-

quently investigated by methods taken from statistical physics. For instance, the appearance of gradient terms were justified by theoretical calculations and models were given for the avalanche-like behaviour and plastic flow. The results presented in the thesis also belong to this field.

Aims of the thesis

1. Dislocations, depending on the external conditions, organise themselves in various patterns. Perhaps the most extensively the persistent slip bands (PSBs) were studied, which evolve during fatigue were studied. By discrete dislocation dynamics simulations even the matrix structure appearing in the first stages of the process was not to be modelled. Meanwhile, many theories worked out for PSB formation are based on the assumption that the energy of interstitial and vacancy type dipoles are different. Discrete simulations always assume linear elasticity and therefore, the mentioned energy difference is zero. A solution can be, if one can step beyond the linear elasticity in the simulations, but for this, the closed form of the new interaction force has to be derived.

2. Dislocations interact via long-range stress fields, which means that for N dislocations the discrete dynamics algorithm has $\mathcal{O}(N^2)$ time complexity. The numerical programme can be made faster by the stochastic method developed by István Groma and Botond Bakó. The central quantity in this theory is the distribution of internal stresses in the crystal. Its form was already determined before, but only in the case, when no external stress is applied to the system. For practical aspects it is necessary to take the external stress into account.

3. According to earlier investigations, it became evident that the dislocation correlations cannot be neglected and they affect many other physical quantities. In order to understand the dynamics of the system in more detail, the precise description of dislocation correlations is needed.

4. A continuum model for single slip was worked out by István Groma and co-workers. The predictions of the model and results obtained by discrete

dislocation simulations are in extraordinary agreement. Unfortunately, its generalisation to multiple slip, which is indispensable for practical aspects, is far not straightforward. The procedure followed at single slip cannot be repeated.

The whole continuum theory was reformulated into a variational approach by István Groma and Géza Györgyi. It is based on a free energy like thermodynamic potential. This method in principle gives the opportunity to generalise the theory to multiple slip. In the thesis we make an attempt to perform this.

5. The relaxation process of dislocations from a random initial state has not been studied in detail before. Although the knowledge about relaxation processes can contribute to the understanding of dislocation avalanches, which are in the centre of interest. During the avalanches, due to external stress, a few dislocations escape from their equilibrium state, and from this point the process can be well approximated by a relaxation. In the thesis, therefore, these kind of processes are also investigated.

Applied methods

The properties of individual dislocations have been known for decades. But the macroscopic behaviour of a dislocation system is crucially affected by the statistical properties of the microstructure. In the 60s, Wilkens proved that dislocations are not located randomly in the crystal. Hence, the detailed description and analysis of such spatial correlations is important not only theoretically, but also in practical aspects.

The currently most popular method to investigate the microstructure is computer simulation. Although three dimensional simulations are already available, their usage is hindered by many aspects, and it has turned out, that two dimensional simulations give equivalent results in many situations. The later, which is far easier to study mathematically, gives the opportunity to deliver analytical calculations, and so, theoretical predictions can directly be checked numerically. In the thesis we follow this procedure, and all our results are supported by two dimensional discrete

dislocation dynamics simulations.

Main results

1. In order to introduce non-linear elasticity, we reformulated the Kröner–Kosevich field theory into a variational model. By giving the form of the introduced enthalpy functional, one simultaneously fixes the relation between the elastic strain and stress. After setting up the enthalpy in the anharmonic case we expressed the dislocation-dislocation interaction force analytically. We succeeded in transforming the obtained convolutional integral into a closed, analytical function, where anharmonicity manifests in an extra term appearing beside the harmonic one. The extra interaction force decays faster than $1/r$ (i.e., it is short-range), and as a curiosity, it explicitly depends on the dislocation inner cut-off radius [1].

   We demonstrated that in the anharmonic case the homogeneous dislocation arrangement becomes unstable, and a pattern with a characteristic length scale forms. This length parameter is proportional to the average dislocation spacing. Discrete dislocation dynamics simulations were performed with the novel interaction force and the results were in complete agreement with the theoretical predictions, i.e., a pattern with a well-defined length scale evolved [1].

2. We determined the distribution of internal stresses in a system subject to external stress. The analytical calculations were performed in the hypothetical monodisperse dipole approximation. The result obtained was in good agreement with the simulations. Summarizing the results, we found that in the large stress region, beside the original $1/|\tau|^3$ type tail, an additional $1/(\tau|\tau|^3)$ type term proportional to the external stress appears. According to numerical studies, the dipoles and multipoles present in the system screen the external stress, resulting an effective stress field, which is approximately half of the original stress [2].

3. Previously, István Groma derived a BBGKY hierarchy for the evolution of different order dislocation densities. We now close the hierarchy at the third

level by applying the Kirkwood superposition approximation, and with this we obtain closed evolution equations for the correlation functions. The resulting equations are very similar to those that describe densities around a screened dislocation. This means that linear response theory (meaning the equivalence of correlations and screened densities) is also valid in dislocation systems. Numerical simulations proved the theoretical predictions in all aspects [3].

4. The continuum theory of single slip can be derived from an appropriate free energy functional. This functional can be generalised to multiple slip by symmetry principles. In the case of symmetric double slip (when the slip planes are perpendicular) the functional contains only one free parameter. The analytical solution of the equations can be given in a simplified case, when the dislocation density is assumed to be constant in space. We found that the induced geometrically necessary dislocation density decays with $1/r^2$. This also means that correlations are short-range. This result, in spite of the approximation applied, fits very well the data obtained from numerical simulations.

5. Numerical studies showed that the relaxation from a random initial state is slow in the sense that many dynamical quantities, such as the averages of different powers of dislocation velocities, decay with a power law. This scaling behaviour starts at a specific time, and lasts until a system size dependent moment [4]. We showed that this feature is the result of the underlying fact, that the velocity distributions at different times obey a scaling law. In multiple slip the relaxation is faster, and the scaling argument does not hold.

Conclusions

- We demonstrated that the dislocation-dislocation correlations have crucial effect on many quantities describing dislocation systems, such as the internal stress distribution, the velocity distribution and evolving patterns. We investigated in detail the dynamics of correlation functions and the multiple slip geometry. Such thorough examination concerning dislocation correlations has not been published in the literature before.

- Dislocations build up non-conservative systems with special dynamics and zero temperature. According to the results of the thesis, numerous methods of statistical physics, after the appropriate modifications, can be applied in the context of dislocations.

Bibliography

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