# Fast-moving dislocations in high strain rate deformation

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# CHAPTER 1

# INTRODUCTION

IT IS A CHALLENGE for any physicist to understand the phenomena of nature in the simplest possible manner. In particular, the materials scientist works his way through the golden triangle of processing, structure and properties of the solid state of matter. It is an exciting journey across many length and time scales ranging from the atomic scale to that of the macro-world. In one of the last Ph.D.-theses of this millennium presented to this university, it seems appropriate to realise that some fundamental ideas only stem from the present century[1].

For instance, the idea of a crystalline state of matter in which the constituent atoms are arranged in regions (grains) of ordered lattices only could be demonstrated experimentally in 1912 with the use of X-rays[2]. By that time dislocations had been observed already, the theory of linear elasticity was developed to a great extent and there were already speculations about their mobility. In the following decades the idea materialised that the plastic deformation of such systems might be caused by *defects* in the lattice. However, what confused the researchers for a longer period of time was the co-existence of the yield drop and of the work-hardening in steel. How could the same defect be responsible for easy glide and in later stages lead to hardening of the crystal? It was not until 1934 that the first arrangement of atoms was proposed by Orowan, Taylor and Polanyi of what we now call an *edge dislocation*[3,4,5], followed somewhat later by the introduction of the so-called *screw dislocation* by Burgers[6]. It is interesting to quote Sir Geoffrey Taylor's view at that time (according to Sir Nevil Mott[7]): "*my paper is a model, not a theory!*" The dislocation was rather a theoretical concept, the use of which had to be validated by experiments much later after World War II.

Now that the basic unit of plastic flow was described, others set out to describe its mobility, at least theoretically. Using discrete models[8,9,10], but also by linear elasticity[11,12], it was established that the resistance to dislocation motion (and hence to plastic deformation) was small at low dislocation velocities, but increased at higher velocities up to the speed of sound. The latter then acts as an upper limit for dislocation velocities. During the late forties and early fifties, the first estimates of the resistance (or *drag* force) were made from the interaction of the moving dislocation with the collective vibrations (phonons) of the crystal lattice[13,14,15]. Later, near the end of the sixties, other contributions to the dislocation drag were identified and treated extensively[16,17].

Meanwhile, it was also recognised that not only the interaction with the lattice itself affects the dislocation motion, but also the interaction with impurities such as solute atoms and precipitates. Theories were developed by Mott, Labusch, Nabarro and Friedel[18–21], and they could explain why the addition of certain types of impurities in a crystal increases its resistance to plastic deformation. Granato[22] later extended these treatments by taking into account the thermally assisted passing of those obstacles.

A prominent contribution to the field of dislocation dynamics is the so-called *Orowan equation*, relating the *macroscopic* strain rate to the mean dislocation velocity. The proportionality is the product of the mobile dislocation density and the mean dislocation velocity. In the old days, however, the emphasis was on the determination of the relation between strain rate and dislocation velocity alone. One of the oldest experimental techniques was based on etch pits. Actually, it dates back to 1855 but was further developed in 1959 by Johnston and Gilman to measure dislocation velocity as a function of externally applied stress[23] . Another milestone in the development of this discipline was the introduction of the transmission electron microscope. This enabled the first *direct* observations of dislocations and their motion in the middle fifties[24,25]. It also permitted many quantitative studies on the subject, and in fact, continue to do so very successfully today (for a review see ref. 26). The body of experimental data that followed the invention of these experimental techniques enabled the development of many of the theories that were mentioned in the previous paragraphs and put them on a quantitative footing.

However, transmission electron microscopy provides information about the *total* dislocation density rather than about the *mobile fraction*. For that reason a complimentary method based on pulsed nuclear magnetic resonance was developed by De Hosson, Kanert and Sleeswijk[27,28] for the study of moving dislocations in metallic and ionic systems up to strain rates of the order of 1 $s^{-1}$. It turned out that from these experiments, three sets of microscopic information about dislocation motion can in principle be deduced: (*i*) the mean jump distance of moving dislocations, (*ii*) the mean time of stay between two consecutive jumps of a mobile dislocation and (*iii*) the mobile dislocation density.

Another important contribution was made by the introduction of the computer as an aid to clarify many phenomena that were not always experimentally accessible, such as the structure of dislocation cores and the motion of the dislocations[29,30]. For instance, in 1966 Foreman and Makin[31] confirmed the theory of Friedel for the interaction of dislocations with point-like obstacles. Rosenfield and Hahn[32] considered *pile-ups* of dislocations. These are arrays of dislocations, where the leading dislocations attain much higher velocities than would be possible under the externally applied stress. It turned out that near the tip of the pile-up the stresses were concentrated to much higher values than for a *single* dislocation (all within the framework of linear elasticity, i.e. excluding core effects).

In more recent years, numerical algorithms have become increasingly sophisticated and, due to the enormous increase in computing power, more accessible to many people. For instance, computational techniques such as the ab-initio calculations, Monte-Carlo method, molecular dynamics, finite elements and so on have found widespread use in many branches of science and engineering. However, even at the current rate of increase in number-crunching power, it is recognised that it will not be possible in the foreseeable future to simulate the deformation of a macroscopic work-piece *directly* from the motion of atoms. It is therefore necessary to split up the important processes according to the time and length scales at which they play a significant role[33]. The processes taking place at the smaller scale then give rise to a certain effective behaviour at a larger scale. For instance, the atomic configuration around a dislocation core directly affects its scattering of lattice waves, thereby contributing to the drag force. On the other hand, when calculating the dislocation velocity due to the resolved shear stress, only this drag force is important, and not so much the precise atomic arrangement.

The connection between different length scales is not always easily made. For instance, in many engineering calculations of plastic deformation, the material is considered to be a continuum. In those cases, the relation between macroscopic stress and macroscopic strain (the *constitutive relation*) is specified, always without taking into account the discrete nature of the carriers of plastic flow, the dislocations. This approach is successful for some applications, but it has the disadvantage that the material behaviour for each type of deformation has to be known in advance. Even for three-dimensional constitutive models, this is hardly ever the case.

On the other hand, some approaches exist nowadays that *do* take into account underlying microstructural processes. This method, called Discrete Dislocation Plasticity (DDP), calculates the deformation of a two-dimensional computational cell by considering the long-range stresses and displacements of edge dislocations moving under influence of an externally applied deformation rate. Furthermore, the interaction between dislocations themselves and with obstacles can explicitly be put into the simulations. One such method was introduced by Van der Giessen and Needleman in 1995[34]. Their method of DDP is not the first to consider moving

dislocations in this manner. However, previous methods only treated dislocations in an *infinite* medium, whereas in their modified DDP it is possible to explicitly take into account the *boundary* conditions in a *finite* medium. The method was compared with a conventional continuum calculation and it was shown that although the overall deformation could be matched, locally there were many stress peaks (that could induce microcracking, for instance), that were not predicted by the continuum approach[35].

One area where this approach is particularly interesting is in the regime of very fast deformation. Measurements at high deformation rates are particularly difficult to perform. The deformation is often localised in very small volumes in which the temperature rises considerably during the process. Sometimes even melting of the material occurs. Recrystallisation due to the temperature rise destroys most of the information of the processes preceding it. For these reasons, the constitutive equations necessary in engineering calculations are often unreliable. Processes where the deformation is fast are quite common in industry. For instance, when a metal plate is perforated, the local rate of strain may exceed $10^3$ $s^{-1}$, even though the overall rate is much lower. Other, more violent examples include the perforation of armour plates by a bullet or the explosive forming of workpieces.

This thesis approaches fast deformation from the small regime of small length scales. Specifically, it focuses on the processes taking place on a single slip system in a single grain of close-packed metal, where the emphasis lies on the fact that the deformation takes place in a very short time span and at very high rates. The method of Discrete Dislocation Plasticity is extended to apply to high deformation rates. One extension is to take into account the limiting velocity to dislocation motion, which is the velocity of sound. This implies taking into account the velocity-dependence of the displacement and stress fields of a moving dislocation. Since the transition of a obstacle-controlled regime to drag-controlled depends on the strength of the obstacles, a physical criterion is introduced to project the obstacle properties from a three-dimensional crystal into the two-dimensional computational cell. Both aspects are treated in Chapter 2.

In Chapter 3 we consider the different regimes of dislocation motion with the focus on the drag-controlled regime. The theories so far hold for low dislocation velocities only, but here we extend this to high velocities, at least for the harmonic contribution of the phonon drag. In Chapter 4 the theories of the previous chapters are actually implemented in a computer code and some examples are shown to demonstrate the method. Chapter 5 deals with the thermal effects of dislocation motion. The methodology is extended to explicitly calculate localisation of heat and its effects on the strengths of obstacles and drag forces. In the past, some estimates of the maximum temperature rise due to plastic flow have been made in the literature, but it has never been calculated exactly. Finally, Chapter 6 looks ahead to an explanation of the temperature rise due to a moving crack and proposes some directions of future research.

## LITERATURE


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