Chapter 6
Plaston—Elemental Deformation Process Involving Cooperative Atom Motion

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6.1 Introduction

There is an ever-increasing demand for structural materials that simultaneously possess high strength and high ductility/toughness. It is, however, very difficult to achieve this in any material because strength and ductility are in general in the trade-off relationship. The material of high strength generally exhibits low ductility/toughness (as in many ceramics) and vice versa. Plastic deformation of crystalline materials usually occurs by shear deformation along a particular crystallographic plane (referred to as slip) so that the shearing of one portion of a crystal occurs with respect to another (by the vector called 'slip vector') upon the crystallographic plane (called 'slip plane'), and such slip is usually (in many cases) carried by a lattice defect called 'dislocation', which is defined as the boundary (line defect) between slipped and unslipped regions on the crystallographic plane (slip plane) (Fig. 6.1). The dislocation can move on the slip plane under the exerted shear stress, displacing one portion of a crystal with respect to another by the vector called 'Burgers vector'. If the stress required to move dislocations is high, the strength of the material is high but the ductility is low because of the difficulty in the dislocation motion. If the stress required to move dislocations is low, in contrast, the strength of the material is low but the ductility is high due to the ease in the dislocation motion.

'Dislocation' is a line defect characterized by the Burgers vector and line vector. By definition, all atoms of one portion of a crystal along the dislocation line are

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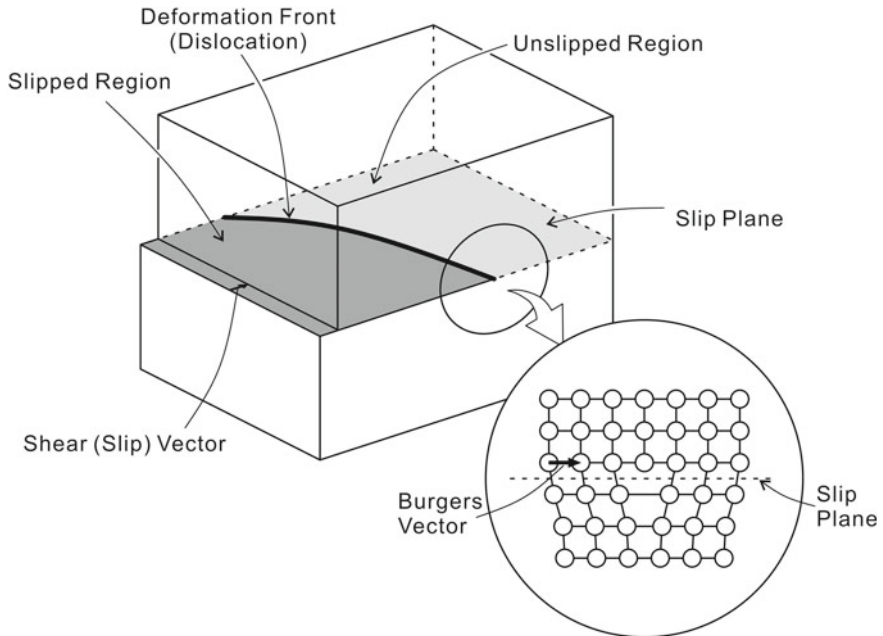
**Fig. 6.1** General description of the elemental process of plastic deformation of crystalline materials with the passage of the deformation front called 'dislocation'

displaced 'uniformly' by an amount determined by the Burgers vector upon the dislocation motion so that the region of the atom displacement occurring in a line (that is dislocation) propagates on the slip plane in the crystal under the exerted shear stress to complete shear (plastic) deformation (Anderson et al. 2017; Nabarro 1967; Friedel 1964; Weertman and Weertman 1964). In this sense, the dislocation is the deformation front that makes cooperative atom displacement, the magnitude of which is determined by the slip (Burgers) vector. One point we should notice here is that the crystal adopts the lowest energy process in plastic deformation, and it is the motion of dislocations that is the lowest energy process in many cases in crystalline materials. The ease of such cooperative atom displacement (along the dislocation line) basically determines the stress necessary to move the dislocation and its mobility, and hence, is closely related to the strength and ductility/toughness of the material. Of course, the strength and ductility/toughness are not determined solely by the intrinsic nature of the crystalline lattice of the material as described above and are dependent also on microstructural features such as grain size and incorporation of alloying elements and other phases (Anderson et al. 2017; Nabarro 1967; Friedel 1964; Weertman and Weertman 1964). The material property has thus been altered in positive ways by tuning these microstructural parameters. One way to break the trade-off relationship between strength and ductility/toughness is to activate a deformation mode different from the dislocation discussed above. Since

Fig. 6.2 Schematic
stress-strain curve for
materials with increased
strength and ductility by
subsequent activation of
different deformation modes
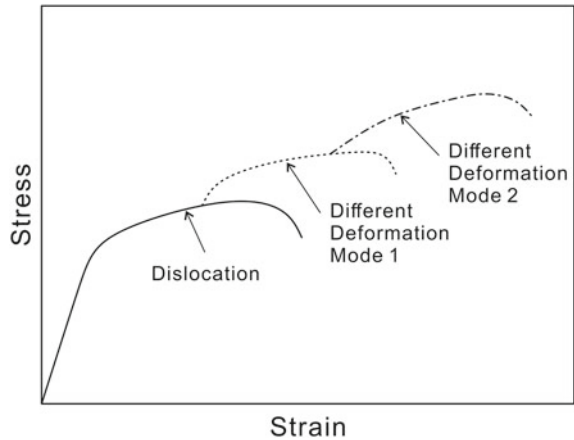
the dislocation is a simple lattice defect that can move relatively easily, the initial plastic flow would be carried by these dislocations. But, if a deformation mode different from 'dislocation' can operate once these dislocations encounter difficulty in their further motion in the course of deformation, both strength and ductility are expected to increase simultaneously (Fig. 6.2). Deformation modes different from the dislocation include dislocations with a different Burgers vector (such as those with the **a+c** Burgers vector in HCP crystals) and those with a different shear mechanism (such as synchroshear (Kronberg 1957) and zonal shear (Kronberg 1959, 1961)), twinning (Read-Hill et al. 1963; Cristian and Mahajan 1995), phase transformation and something else (related to grain boundary motion and so on) (Anderson et al. 2017; Nabarro 1967; Friedel 1964; Weertman and Weertman 1964). TWIP and TRIP steels (Frommeyer et al. 2003; Cooman et al. 2018) as well as, more recently, high-entropy alloys with the FCC structure (Otto et al. 2013; Gludovatz et al. 2014) are some nice examples, in which simultaneous achievement of high strength and high ductility is realized by inducing the activation of different deformation modes following the starvation of the primary mode of dislocation.

It seems very important to understand how we can activate not only the primary deformation mode (the simple dislocation) but also the secondary (and tertiary) deformation mode(s), in terms of stress level/state, crystallographic orientation, grain size and orientation relationships with neighboring grains and so on for the development of structural materials with high strength and ductility/toughness. We call all these deformation modes including the primary dislocation 'plaston' (see the reason below) and discuss the importance of the understanding of the activation of various plastons for achieving high strength and ductility/toughness.

6.2 Nucleation and Motion of Plastons (Possible Deformation Modes) Under Stress

Crystalline materials generally contain grown-in dislocations that are introduced during solidification (and forming as well) unless otherwise some particular care is taken. Grown-in dislocations are in general simple dislocations that can move at the lowest stress levels (among the available deformation modes in the material), since they are introduced most easily in order to relieve internal stresses developed during solidification. If the stress level for the dislocation motion is too high (as in many brittle materials), the material cracks instead of introducing dislocations. Upon plastic deformation, these grown-in dislocations move and multiply new dislocations once external stress sufficiently high enough to move them is applied to the material. This is because these dislocations are the weakest parts of the material under stress such that cooperative atom displacements along the dislocation line can occur most easily, when compared to otherwise perfect portions without any lattice defects. Multiplication of dislocations from these grown-in dislocations is what usually occurs in most bulk crystalline materials during deformation. As the specimen size becomes smaller down to sub-micron meter sizes, however, the possibility to find out grown-in dislocations in the specimen becomes lower, such that plastic deformation occurs by the nucleation of new dislocations and their subsequent motion (but not by multiplication of dislocations from the pre-existing grown-in dislocations), as have frequently been seen in whisker and micro- and nano-pillar specimens (Uchic et al. 2004; Okamoto et al. 2013, 2014, 2016; Chen et al. 2016; Zhang et al. 2017; Kishida et al. 2018, 2020; Higashi et al. 2018). When there is no available pre-existing (grown-in) dislocation at the beginning of plastic deformation, the stress level for deformation is known to be quite high from experiments with whisker and micro- and nano-pillar specimens.

One of the typical examples that are accompanied by the nucleation of dislocation during plastic deformation is shown in Fig. 6.3 for the case of micropillar compression tests made for two different orientations of single crystals of Ti_3Al with the DO_{19} (ordered HCP) structure. Because of the brittleness of this particular intermetallic together with the small specimen size, it is fairly a safe assumption that there are virtually no grown-in dislocations available at the beginning of plastic deformation. Two different deformation modes are activated depending on crystal orientation. Pyramidal **a+c** ({$11\bar{2}1$}<$11\bar{2}6$>) slip with the highest CRSS value in the bulk is observed to operate in the whole specimen size range investigated for the [0001] orientation, while pyramidal **a+c** ({$11\bar{2}1$}<$11\bar{2}6$>) slip is replaced by prism **a** ({$1\bar{1}00$}<$11\bar{2}0$>) slip as the specimen size decreases for the [$2\bar{1}\bar{1}0$] orientation with the slip system transition occurring at around 6 μm. In view of the fact that grown-in dislocations, if exist, are expected to have a Burgers vector **b** $= 1/3$<$11\bar{2}0$>, plastic deformation is believed to occur by the nucleation of dislocations and their subsequent motion. This is believed to be the case not only for the [0001] and [$2\bar{1}\bar{1}0$] oriented micropillar specimens where **a+c** dislocations are activated but also for smaller micropillar specimens with the [$2\,\bar{1}\bar{1}0$] orientation, since the CRSS (critical resolved shear stress) values for prism **a** slip obtained in micropillars are considerably
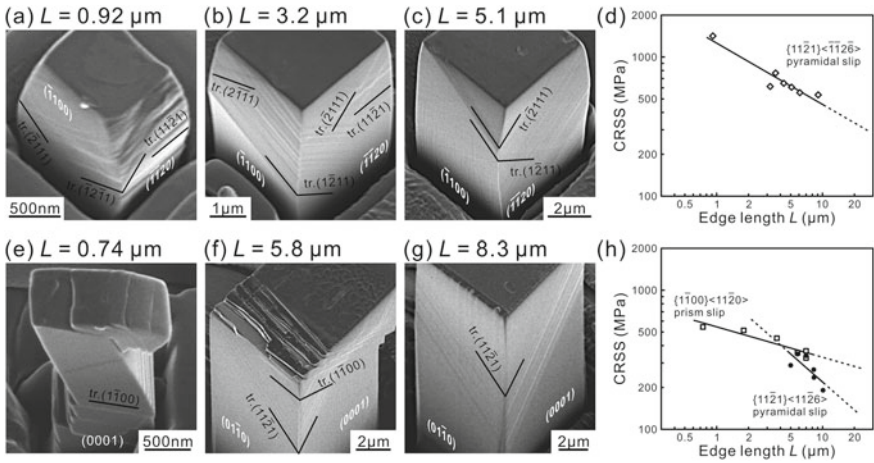
Fig. 6.3 Micropillar compression tests on **a–d** [0001]- and **e–h** [$2\bar{1}\bar{1}0$]-oriented Ti_3Al single crystals

higher than that for the bulk. If we assume that the yield stress (CRSS) observed in micropillar compression tests is well correlated with the nucleation stress for dislocations, the nucleation stress for dislocations of a particular slip system obviously varies with the specimen size. The fact that the operative deformation mode changes with the specimen size even with the same orientation (the slip system transition for the [$2\bar{1}\bar{1}0$] orientation in Ti_3Al) clearly indicates that the selection of operative deformation mode is the subject that is determined by stress level/state, crystallographic orientation, specimen size (grain size) and so on. Although the above example deals with dislocations with different Burgers vectors (**a** and **a+c**), it is obvious that other deformation modes including twinning, phase transformation and something else (related to grain boundary motion and so on) can all be subject to be considered for the nucleation under stress as deformation modes to carry plastic strain, as will be detailed in the next section.

When deformation is made along a fixed path (as in uniaxial tensile and compression tests), lattice instability starts to occur as the stress (strain) increases so that the saddle (bifurcation) point is passed (Fig. 6.4). The lattice instability may be evaluated, for example, by the positivity of elastic stiffness constants (Born's lattice instability criteria) (Yashiro 2012). If this occurs in some local area of the specimen (as can happen due to stress concentration at (even atomic) steps on the specimen surface), the area of such lattice instability is considered to contain atoms that are cooperatively exited and that change their arrangement energetically suitable to the exerted stress/strain state (cooperative atom displacement). Such a change in the atomic arrangement under stress produces a dislocation in some cases and other deformation carriers (twinning, phase transformation and so on) in other cases. We believe this is the nucleation of plastons (Fig. 6.5a). The nucleation of plastons may occur at steps on the specimen surface (more precisely, on the corner edge of the specimen) to avoid any significant constraint from the surroundings in the case of
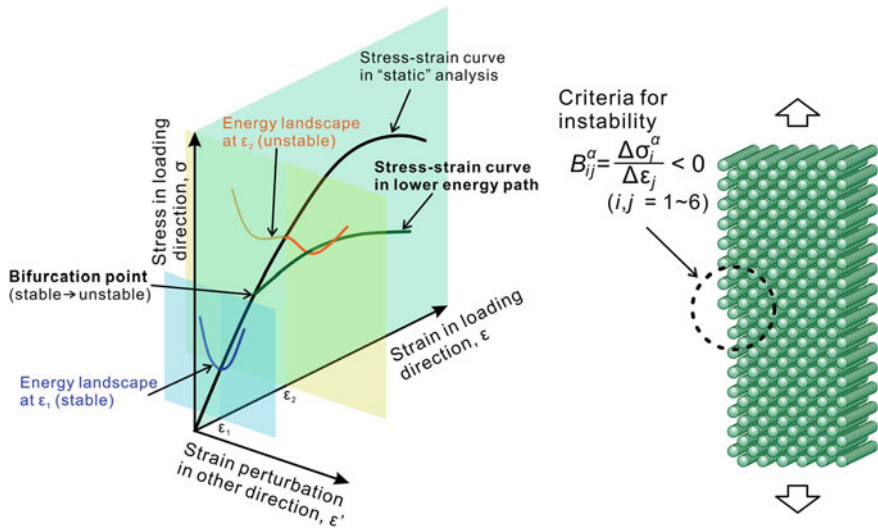
Fig. 6.4 Lattice instability occurring during deformation along a fixed path at high stress levels, where the positivity of elastic stiffness constants is violated (after Yashiro (2012))
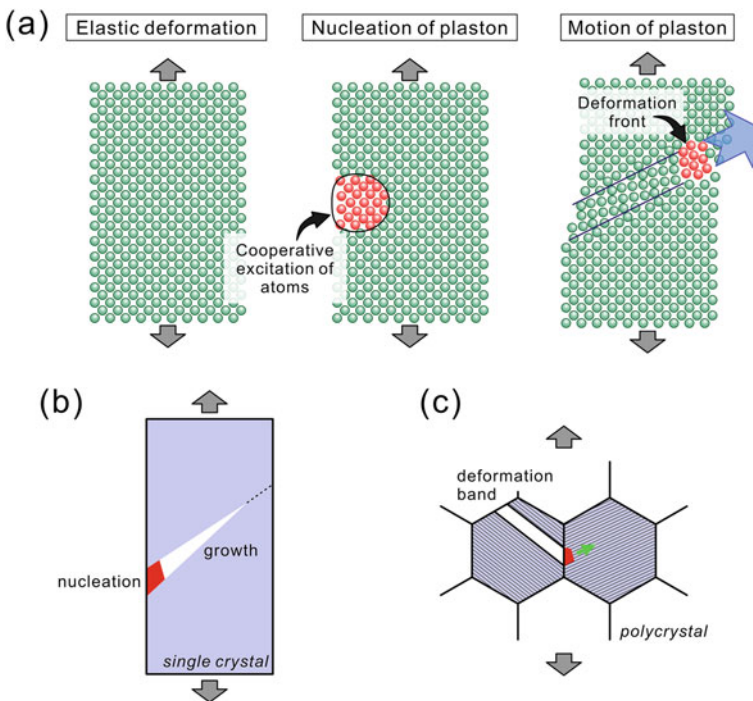
Fig. 6.5 **a** General schematics of nucleation and motion of plaston. Nucleation of plaston in **b** single crystal and **c** polycrystals

single-crystalline micro- and nano-pillars (Fig. 6.5b). But, the nucleation of plastons at the grain boundary must be more important when considering bulk polycrystalline materials in practical use for deformation propagation across the grain boundary (Fig. 6.5c). We also believe that the deformation mode (plaston) selected among possible deformation modes must be that which involves the atomic process of the lowest energy depending on stress level/state, crystallographic orientation, specimen size (grain size) and so on for a particular material. Their subsequent motion must also be dependent on stress level/state, crystallographic orientation, specimen size (grain size) and so on, so that the deformation mode difficult to move may not be selected to contribute to the plastic flow of the material. Atoms that are cooperatively excited are generated locally under stress and they change the atomic arrangement to energetically fit with the exerted stress/strain state, crystallographic orientation, orientation relationship with neighboring grains (in the case of polycrystals) and so on during deformation, generating (nucleating) the deformation carries (plastons), and they spread as a line defect (in many cases, along a particular crystallographic plane) in the crystal to carry plastic strain. We call these deformation carriers 'plastons'. We have to think of both the nucleation and motion of these plastons, as in the case of dislocations. Needless to say, these deformation carriers are not necessarily dislocations but can be others.

6.3 Cooperative Motion of Atoms in Plastons

When grown-in dislocations are available, they move and multiply new dislocations once external stress sufficiently high enough to move them is applied to the material (Anderson et al. 2017; Nabarro 1967; Friedel 1964; Weertman and Weertman 1964). In this case, these dislocations are the weakest parts of the material under stress such that cooperative atom displacements along the dislocation line can occur most easily. In this way, simple dislocations are plastons (deformation carriers) that carry plastic flow at least in the early stages of plastic deformation in many conventional metallic materials (the inset of Fig. 6.1).

When these grown-in dislocations are not available (as in nano- and micro-pillars, ultrafine-grained materials and hard and brittle materials), the nucleation of plastons (deformation carriers) is needed to initiate plastic flow so that atoms that are cooperatively exited change their arrangement energetically suitable to the exerted stress/strain state (cooperative atom displacement). The simplest way to achieve this may be to nucleate simple dislocations. But, if this is not possible (for example, by the reason of the unfavorable crystal orientation, unfavorable orientation relationship with neighboring grains, too high stress level for simple dislocations due to work-hardening and so on), plastons (deformation carriers) different from simple dislocations will be selected at stress levels higher than that for simple dislocations. These plastons nucleated at higher stress levels include dislocations with a different Burgers vector (such as those with the **a+c** Burgers vector in HCP crystals) and those with a different shear mechanism (such as synchroshear (Kronberg 1957) and

zonal shear (Kronberg 1959, 1961)), twinning (Read-Hill et al. 1963; Cristian and Mahajan 1995), phase transformation and something else (related to grain boundary motion and so on)) (Anderson et al. 2017; Nabarro 1967; Friedel 1964; Weertman and Weertman 1964).

Here, we take an example of twinning as a plaston to explain cooperative atom displacement occurring in the nucleation and in the propagation as the deformation front during plastic deformation. In deformation twinning in HCP metals, the nucleation of a twin is known usually to occur at the surface or at the grain boundary. The nucleation of a twin may occur in some area that contains atoms cooperatively exited and change their arrangement energetically suitable to the exerted stress/strain state, crystallographic orientation, specimen size (grain size) and so on for a particular material. This is discussed in detail by Tanaka and Togo in a different chapter of this book and will be briefly described in the next section. Then, the area propagates as a plaston (deformation front) making a complicated cooperative atomic motion as frequently called 'shuffling', as this cannot be expressed with a single displacement vector (Fig. 6.6b). This occurs because HCP metals are 'diatomic' having two atoms at each of the primitive hexagonal lattice points, in contrast to the case of FCC and BCC metals, in which only a single atom is allocated to each of the face-centered and body-centered cubic lattice points ('monoatomic'), respectively. Displacements of atoms in the plaston (deformation front) are thus the same for all atoms in FCC and BCC metals, coinciding exactly to the Burgers vector of the 'twinning' partial dislocation. However, displacements of atoms in the plaston (deformation front) in 'multi-atomic' materials (with multiple atoms at each lattice point) generally differ from atom to atom and they do not generally coincide with the displacement vector of the relevant lattice points. In this case, the displacement vector of the relevant lattice
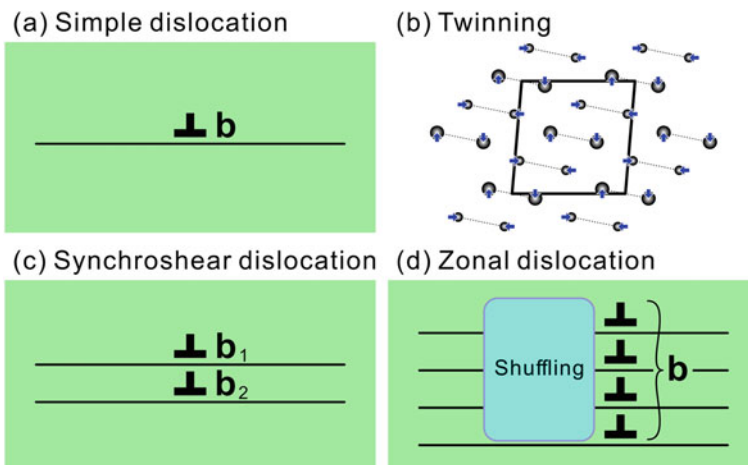
Fig. 6.6 Plastons of different types; **a** simple dislocation, **b** twinning, **c** synchroshear dislocation and **d** zonal dislocation. Compare the simple dislocation in the inset of Fig. 6.1

points is often assigned as the Burgers vector of the twinning dislocation for convenience. In this sense, the 'twinning dislocation' in 'multi-atomic' materials is quite different from that in 'monoatomic' materials. The fact that all atom displacements cannot be described simply with the Burgers vector indicates clearly that propagation of the plaston (deformation front) indeed includes the cooperative motion of atoms of the lowest energy under stress.

There are some particular dislocations that may involve a volume for cooperative atom motion probably larger than that for simple dislocations during their nucleation and motion. The way of cooperative atom motion for these dislocations is necessarily more complicated because the shearing process with these dislocations involves a few to several successive parallel atomic planes, in contrast to simple dislocations for which the shearing process involves a single atomic plane. The 'synchroshear' dislocation involves multiple (two, in many cases) successive parallel slip planes displaced synchronously along different (Burgers) vectors on each of the planes so as to give the displacement corresponding to the sum of the all vectors as a whole (Fig. 6.6c). This concept was first predicted for basal slip in alumina (Kronberg 1957), then for slip in compounds of the Laves phase (Chu and Pope 1984; Hazzledine and Pirouz 1993). The concept was proved experimentally first in transition-metal silicides with the C40 structure (Moriwaki et al. 1997; Inui et al. 1998) and then for basal slip in Laves-phase compounds (Kumar and Hazzledine 2004). The 'zonal' dislocation involves much more parallel slip planes called 'shear zone' in which atoms in the slab move non-uniformly but cooperatively by varying amounts (Fig. 6.6d). A typical example is prism **a+c** slip in HCP metals, as detailed in the past (Kronberg 1961). Slip in sigma-phase compounds is another example, in which atomic rings in the Kagome layers are forced to make a rotation in a cooperative manner. This was proved experimentally to occur for {110}<001> slip recently (Kishida et al. 2020).

We believe that the nucleation and motion of plastons are important also in bulk metallic glasses [for example, (Kumar et al. 2010)]. In bulk metallic glasses, plastic deformation is known to occur by the passage of the so-called shear zone (Ogata et al. 2006). Cooperative atom motion must occur at the front of the shear zone to energetically fit the exerted stress, sometimes generating another glass structure of the lower energy, referred to as rejuvenation (Meng et al. 2012).

All these indicate that the cooperative and complicated atom motion occurs in general in the deformation front under stress in many different materials. Of importance to remember is that such cooperative and complicated atom motion is sometimes energetically favored under certain circumstances in particular materials. It is thus very important to consider how we can control the occurrence of such cooperative and complicated atom motion.

6.4 Origin of Cooperative Atom Motion in the Nucleation of Plastons

Plastons that make an energetically favorable cooperative atom motion will be nucleated depending on the exerted stress/strain state, crystallographic orientation, orientation relationship with the neighboring grain and specimen size (grain size), as discussed above. We now show how the selection of deformation mode (carrier) would be made by taking an example of deformation twinning in HCP metals only briefly, since this is discussed in detail by Tanaka and Togo (Tanaka and Togo this book) in a different chapter of this book. As discussed in Sect. 6.2 of this paper, the nucleation of plastons will be made in some local area of the specimen in which lattice instability occurs as a result of high stress/strain. Then, the question is how such lattice instability occurs. Tanaka and Togo have indicated that phonon instability occurring as the shear stress/strain increases triggers the cooperative atom rearrangement accompanied by crystal symmetry breaking, resulting in $\{10\bar{1}2\}$ twinning in Ti in their first-principles calculations. According to them, the cooperative atom motions during shuffling are correctly predicted. The selection of $\{10\bar{1}2\}$ twinning as the plaston to carry plastic strain occurs of course only when the crystal is oriented favorably for its occurrence. Otherwise, the selection of other modes will be energetically more favored. Although yet to be proved by first-principles calculations, slip with dislocations of the particular type will be similarly selected as the lowest energy process driven by lattice instability depending on crystal orientation (the magnitude of shear stress acting on the relevant deformation modes). Of importance to note is that the selection of plaston is made as the lowest energy process driven by lattice instability that triggers the cooperative atom rearrangement, depending on the exerted stress/strain state, crystallographic orientation, orientation relationship with the neighboring grain and specimen size (grain size).

6.5 Applications of the Concept of Plastons to the Improvement of Mechanical Properties of Structural Materials

Structural materials are used usually in the form of polycrystals mostly for economic reasons, except for some examples such as Ni-based superalloys used as turbine blades. This means that the concept of plastons should be applied effectively to polycrystalline materials in practical use for the improvement of mechanical properties of existing structural materials and for the development of new materials with high strength and high ductility/toughness. Although plastons are explained and discussed mainly with single crystals for ease of understanding in this paper, the nucleation of plastons at the grain boundary has to be taken into account (Fig. 6.5c). When deformation propagates across the grain boundary in polycrystalline materials, the nucleation of deformation mode (carrier) occurs in a new grain adjacent to

the already-deformed grain or at the grain boundary between the two grains so as to satisfy strain compatibility across the grain boundary. Which deformation mode is selected upon deformation propagation across the grain boundary would be determined by the stress level/state and crystallographic orientation of the new grain (magnitude of shear stress), orientation relationship between the two adjacent grains (strain incompatibility), stress level/state of the grain, grain size and so on. Generally speaking, if the grain size is large on the milli-meter order, the deformation mode with the lowest CRSS (simple dislocations in most cases) is usually selected, unless there is some special orientation relationship among grains. In this case, slip carried by simple dislocations is observed in all grains throughout the specimen. This is actually the main cause of the low formability of many HCP metals, in which deformation modes with the **c**-axis component are hardly activated because of the higher CRSS values. However, there is an increasing possibility to activate deformation modes other than simple dislocations as the stress level increases, for example, by reducing the grain size (ultra fine-grained materials) and by strengthening through solid-solution hardening (high-entropy alloys). If some different deformation modes are activated as the stress level increases, following the primary slip with simple dislocations, high strength and high tensile ductility are expected to simultaneously be achieved (Fig. 6.2).

TWIP and TRIP steels (Frommeyer et al. 2003; Cooman et al. 2018) and high-entropy alloys (Otto et al. 2013; Gludovatz et al. 2014) are a good example for this. In addition to slip by simple dislocations, partial dislocations to produce twins and/or ε-martensite are activated at high stress/strain levels, leading to high strength and ductility. Obviously, the stacking fault energy and the relative energy difference between the relevant FCC and HCP phases are parameters to control the activation of partial dislocations to produce twin and/or ε-martensite, as the twinning stress, for example, has been believed to correlate positively with the stacking fault energy (Venables 1961). Of interest to note is that the opposite trend (negative correlation between the twinning stress and stacking fault energy) is recently reported (Laplanche et al. 2017), indicating that there is still enough room to investigate how we can activate partial dislocations to produce twins and/or ε-martensite in FCC-based alloys.

Ultra fine-grained materials may be another good example of this. As the grain size decreases, the strength of these ultra fine-grained materials is increased, but at the same time, the ductility generally decreases catastrophically. However, once deformation modes other than slip by simple dislocations are activated, the improvement of ductility is sometimes observed (Tsuji et al. 2020). The activation of partial dislocations to produce twins and/or ε-martensite, other dislocations with different Burgers vectors, disclinations and grain boundary sliding may contribute to the improvement of ductility of ultra fine-grained materials. An example is shown for ultra fine-grained Mg with the HCP structure in Fig. 2 of (Tsuji et al. 2020). Pyramidal **a+c** slip is observed to operate, in addition to primary basal **a** slip, once the grain size is reduced below 1∼2 μm, significantly improving the tensile ductility. This is an example showing how a high-stress state achieved by reducing the grain size can activate a deformation mode other than simple dislocations. The change in the *c/a*

axial ratio by alloying is known to be effective to induce deformation modes with the axis component in HCP metals (for example, Al additions to Ti, and Zn and rare-earth element additions to Mg).

However, almost nothing is known about how we can effectively activate these additional deformation modes at high stress/strain levels in a general sense. Although some examples are shown above, the effects of orientation relationships among adjacent grains (texture) including those with the hard secondary phase grains have remained largely unknown in spite of the primary importance for actual structural materials in practical applications. It seems very important to investigate how we can effectively activate these additional deformation modes with the concept of plastons as outlined in this paper for the improvement of mechanical properties of existing structural materials and the development of new materials with high strength and high ductility.

6.6   Conclusions

Plaston is defined as a defect that is nucleated and propagates as a line defect of the deformation front to carry plastic flow under shear stress. The nucleation of plastons occurs in some local area of the specimen of lattice instability such that atoms in that local area are cooperatively exited and change their arrangement energetically suitable to the exerted stress/strain state (cooperative atom displacement) to form a plaston of the lowest energy. The selection of a plaston of a particular type among many different plastons depends on stress level/state, crystallographic orientation, specimen size (grain size) and so on. The importance of the understanding of the activation of various plastons is discussed.

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