

# An approach to the plasticity of hcp metallic crystals in terms of their structure dynamics

Giuseppe Caglioti, Dipartimento Ingegneria Nucleare e  
Istituto Nazionale Fisica Materia, Politecnico di Milano, 20133 Milano

## Abstract

*From the phonon dispersion relations of a crystal, via the interatomic or interplanar force constants, interesting information can be extracted on the mechanical behavior of the crystal itself and, in particular, on the slip systems of Mg and other hcp metals.*

*It is found that, according to calculations of the Peierls stresses and Peierls energies based on lattice dynamics, not only for Zr, but also for Mg, prismatic slip should prove to be almost as favorable as the basal slip. This circumstance might help to explain the sudden onset, at 220°C, of pyramidal slip in Mg, observed in 1959 by H. Asada and H. Yoshinaga.*

*Finally, always with reference to Mg, it is suggested that in order to assess the relative importance of the basal and prismatic slip systems on the one hand, and e.g. the  $(a+c) 1/3 [01\bar{1}1] [\bar{1}\bar{1}23]$  pyramidal slip system on the other hand, one should compare the information already extracted from the dispersion relations along the principal symmetry directions of its crystal structure with the analogous information obtainable from the dispersion relations along reduced symmetry directions such as  $[\bar{1}\bar{1}23]_L$  and  $[01\bar{1}1]_T$  polarized along  $[\bar{1}\bar{1}23]$ . However, to our knowledge, these neutron spectrometry measurements have not been performed yet.*

## Riassunto

Dalle relazioni di dispersione di un cristallo, attraverso le costanti di forza interatomiche o interplanari, è possibile estrarre informazioni sul comportamento meccanico del cristallo stesso e, in particolare, sui sistemi di slittamento del Mg e di altri metalli a struttura esagonale compatta.

Secondo calcoli degli sforzi e delle energie di Peierls basati sui dati di dinamica della struttura cristallina, il sistema di slittamento prismatico dovrebbe essere favorito quasi quanto il sistema di slittamento basale, non soltanto per lo Zr ma anche per il Mg. Questo fatto potrebbe rendere conto dell'improvviso apparire del sistema piramidale di slittamento del Mg, quale osservato a 220°C da H. Asada and H. Yoshinaga nel 1959.

Infine, sempre con riferimento al Mg, si suggerisce che per valutare la competitività tra i sistemi di slittamento basale e prismatico da un lato e, ad esempio, il sistema piramidale di slittamento  $(a+c) 1/3 [01\bar{1}1] [\bar{1}\bar{1}23]$  dall'altro lato, occorrerebbe confrontare le informazioni già utilizzate sulle relazioni di dispersione nelle principali direzioni di simmetria del cristallo con le analoghe informazioni desumibili a partire dalle relazioni di dispersione

lungo direzioni quali  $[\bar{1}\bar{1}23]_L$  e  $[01\bar{1}1]_T$  con polarizzazione  $[\bar{1}\bar{1}23]$ . Tuttavia sembra che misure di spettrometria neutronica in questo senso non siano ancora state eseguite.

## INTRODUCTION

The objective of this contribution is to show that relevant information on the mechanical properties of metals can be extracted, via the interplanar force constants (Fig. 1), from the dynamics of atoms in crystal structures.

In particular, for the hexagonal close packed metallic crystals, a correlation is suggested between the interplanar force constants of the structure dynamics and the dislocation mobility along competing (basal prismatic and/or pyramidal) slip systems (Fig. 2).

Here, results published long time before the informatic revolution are critically reviewed and additional neutron spectroscopy measurements are proposed in order to assess the relative importance of the pyramidal slip systems of magnesium with respect to the thoroughly investigated basal and prismatic ones.

## FROM THE DYNAMICS OF CRYSTAL STRUCTURE OF HCP METALS TO THEIR MECHANICAL PROPERTIES

At the atomic scale, the dynamics of a crystal, although involving an astronomic number of degrees of freedom -  $6N$  for a hcp crystal whose  $N$  trigonal unit cells contain 2 atoms each -, can be handled simply thanks to the crystal periodicity, which allows to deal only with the 6 degrees of freedom of a single unit cell: due to the translational symmetry, any cell is representative of the whole crystal structure because of the translational invariance of the structure itself. The study of crystal dynamics can be conveniently referred to the Fourier or reciprocal space-time: under the assumption that neighbor atoms are coupled one to another one by harmonic forces, the atomic displacement is expanded in terms of a linear superposition of elementary, collective, oscilla-

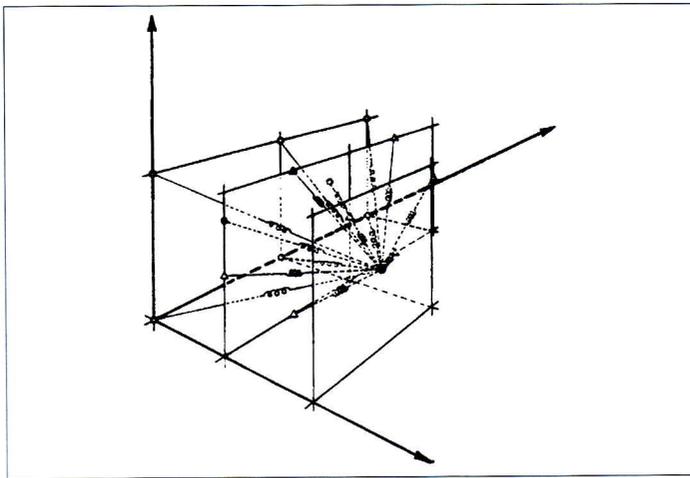


Figure 1: The interplanar force constants between first nearest neighbor (100) planes and second nearest neighbor (100) planes of a face center cubic (fcc) crystal. They are obtained by summation of the interatomic force constants coupling neighboring atoms on the above planes, as indicated.

tory displacements - the normal modes of vibration - . The Fourier amplitudes at equilibrium, the frequencies and the polarization unit vectors of the normal modes depend on the propagation wavevector  $\mathbf{q}$  and branch index  $j$ .  $\mathbf{q}$  is defined in the first Brillouin zone of the reciprocal space and takes  $N$  possible values ; its modulus,  $q$ , is the number of oscillation wavelengths per unit length.  $j$  labels the nature - longitudinal, transverse, acoustic, optic, etc - of the 6 branches exhibited by the hcp metals. Each normal mode can be envisaged as a harmonic oscillator whose frequency,  $\omega$ , depends on the wavevector  $\mathbf{q}$  and the branch index  $j$ . The dispersion relation  $\omega = \omega(\mathbf{q}, j)$  conveys important information on the dynamic features of the crystal. (Fig. 3)

Let's visualize some normal modes whose wavevectors  $\mathbf{q}$  lie along specific crystal symmetry directions such as the [0001], orthogonal to the basal planes and [0110], along the projection of the basic vector on the basal planes.

These modes describe harmonic oscillations of crystal planes as whole units. For instance, every  $\mathbf{q}$  along the [0001]L and [0001]T branches supports oscillations of the basal planes coherently organized according to vibrational waves propagating along the hexagonal axis and polarized along it and along the basal plane respectively:  $q_c$  is a measure of the relative phase of contiguous cells participating to the collective oscillation.

For the special value  $\mathbf{q} = \mathbf{0}$ , at the origin of the reciprocal space and at the center of the Brillouin zone(s), the [0001]LO (Longitudinal Optic) mode corresponds to contiguous cells vibrating in phase ( $q_c = 0 \text{ mod } 2\pi$ ) and contiguous basal planes vibrating with opposite phases along the direction of the hexagonal axis. Clearly this vibrational mode is controlled by interplanar force constants associated to interplanar springs which must be stretched in order to trigger cleavage. We'll come back in a moment to these interplanar springs

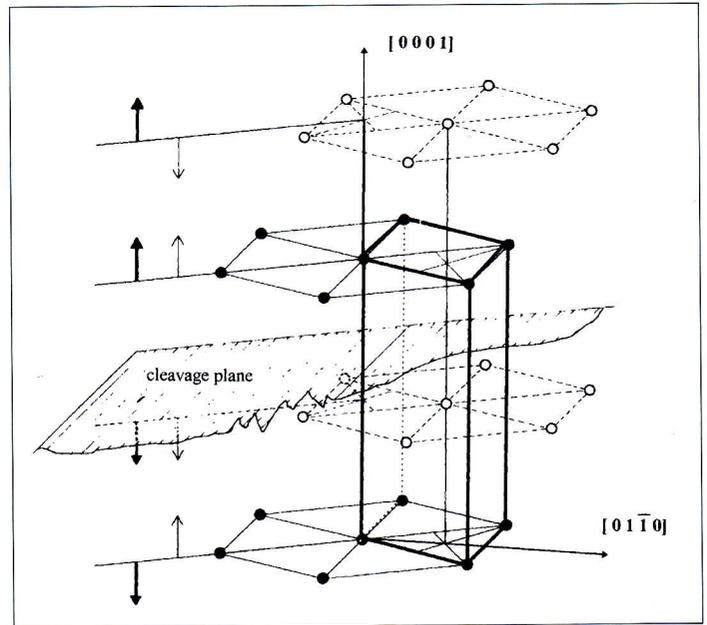


Figure 2: The hexagonal close packed (hcp) crystal structure. Each trigonal unit cell (bold line) contains two atoms. The [0001] and the [0110] symmetry directions are indicated. The light arrows visualize the polarization unit vectors of the [0001] LO mode at  $q = 0$ , while the bold arrows visualize the cleavage mode, splitting eventually the crystal into two half-crystals across the cleavage plane.

in order to propose a correlation of their compliance with cleavage of zinc. Actually zinc cleaves easily. If one immerses a single crystal of zinc in liquid nitrogen and extracts it after one minute, a little stroke of a hammer against an old Gillette razor blade of the Sixties leaning parallel to the basal planes of the crystal will be sufficient to cleave it into two half-crystals separated by shining atomic flat mirrors.

Similarly, always for  $\mathbf{q} = \mathbf{0}$ , the [0001]TO (Transverse Optic) mode corresponds again to contiguous cells vibrating in phase and contiguous basal planes vibrating with opposite phases but, in this case, along a direction parallel to the basal plane. This vibrational mode is controlled by interplanar force constants associated to interplanar springs which must be stretched in order to produce basal slip.

As for any harmonic oscillator, the above force constants are proportional to the squares of the corresponding vibrational frequencies. Furthermore, at equilibrium, the lower the frequencies (and the associated force constants), the higher are the mean square amplitudes of the associated normal modes.

Consequently, for instance, the comparatively low value of the frequency of the [0001]TO mode of zinc at  $\mathbf{q} = \mathbf{0}$  is likely correlated with the strongly favored (1120)[0001] slip system of this metal, characterized by an axial ratio  $c/a$  much higher than the ideal one [1].

The frequency vs. wavevector dispersion relations of the normal modes of vibration are measured by neutron

spectroscopy. As mentioned above, the dispersion relations along symmetry directions disclose access to the interplanar force constants.

At the Ispra-1 reactor, thirty five years ago, we measured the frequency vs wavevector phonon dispersion relations along the  $[0001]$  and  $[01\bar{1}0]$  directions of zinc [1].

At that time, although the interatomic and interplanar force constants of zinc and other "simple" metals were becoming available via the measured dispersion relations, the usual approach toward an understanding of the mechanical properties of matter was yet based on continuum mechanics. Instead we utilized our results e.g. within the frame of a model expressly developed in order to evaluate the Griffith surface energies for (brittle) fracture, of zinc - and other crystals as well - [2], from the  $\omega(\mathbf{q},j)$ 's and the associated interplanar force constants.

In particular, we tentatively correlated the tendency of zinc to cleave at low temperature along the basal plane with the circumstances that:

- the interatomic force constant between first nearest neighbors in the basal plane, equal to  $25 \times 10^4$  dyne/cm (as deduced from the analysis of the vibrational frequen-

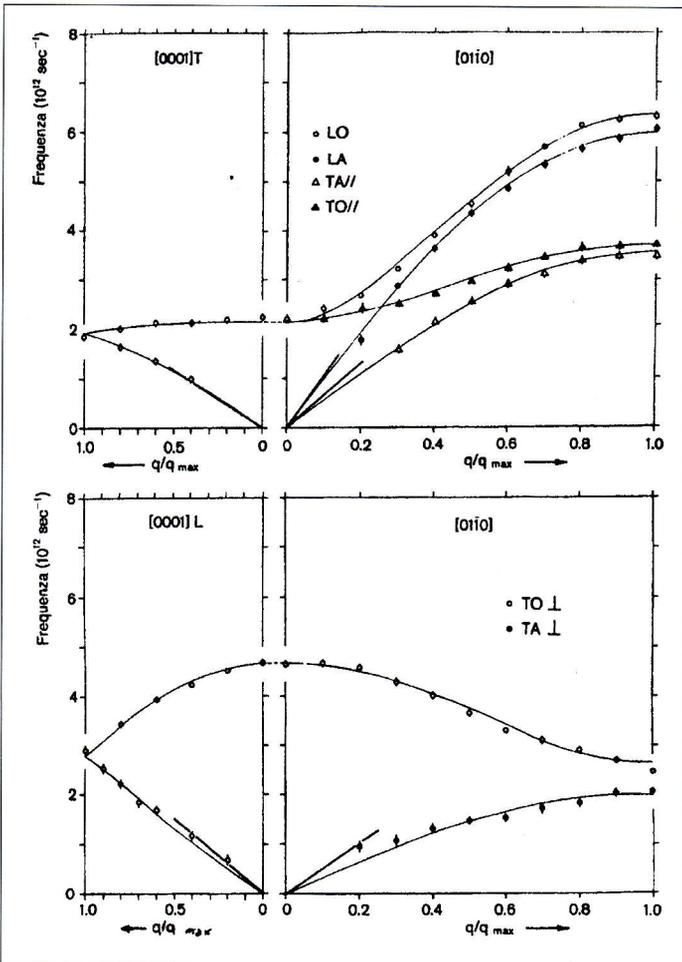


Figure 3: The frequency vs. wavevector dispersion relations of zinc at room temperature along the symmetry directions  $[0001]$  and  $[01\bar{1}0]$ .

cies of the comparatively stiff  $[01\bar{1}0]$ L and  $[01\bar{1}0]$  T// acoustic and optic branches which involve vibration in the basal plane only) turns out to be at least five times larger than any other force constant among other atom pairs in the crystal. The high stiffness of the spring coupling nearest neighbors in the basal plane confers a strong individuality to this plane in comparison with other crystallographic planes, as well as a remarkable anisotropy to the whole crystal;

- to a difference with respect e.g. to Mg (Fig. 4), in Zn the frequency  $\omega[0001]$ LO of the longitudinal optic mode at  $\mathbf{q} = \mathbf{0}$  is comparatively lower than the maximum (Debye) frequency of the crystal. Correspondingly, at equilibrium, as a consequence of the comparatively high compliance of this specific oscillator, the mean square amplitudes of the vibration of contiguous basal planes oscillating with opposite phases along the hexagonal axis are already comparatively large. In other words, the crystal dynamics of zinc is inherently *soft* against cleavage.

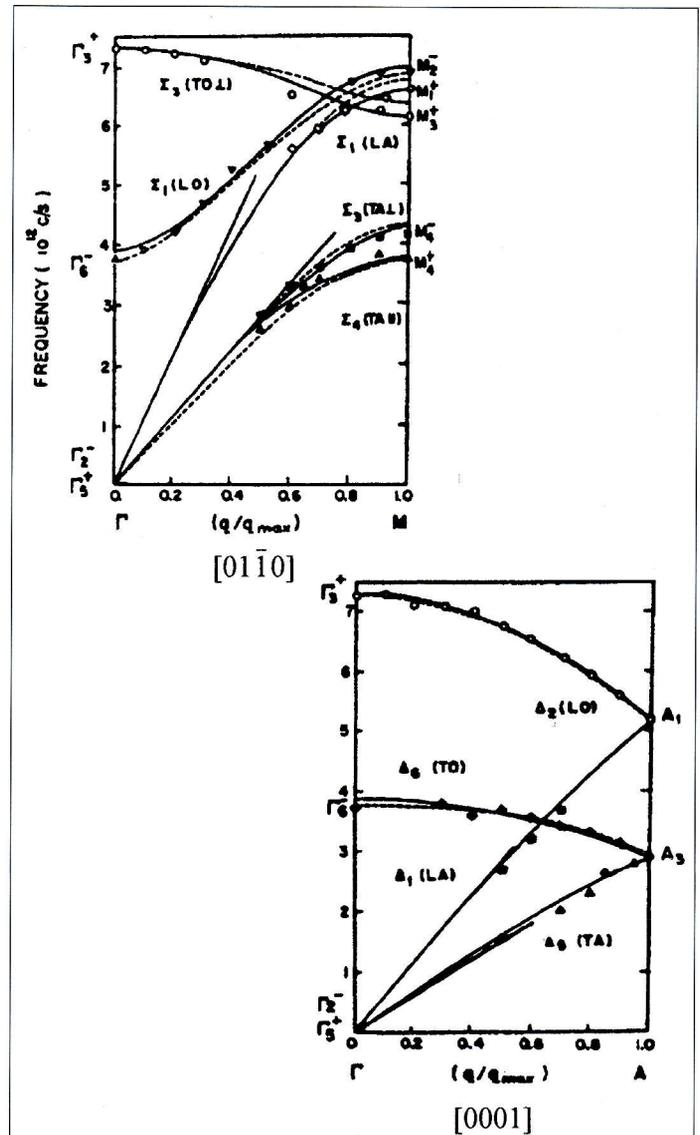


Figure 4: The frequency vs. wavevector dispersion relations of magnesium at room temperature along the symmetry directions  $[0001]$  and  $[01\bar{1}0]$ .

## THE SLIP SYSTEMS OF HCP METALS: REMARKS AND PERSPECTIVES

Twenty five years ago, again taking advantage of the results obtained on the dynamics of crystal structures from neutron spectroscopy, we modified a model based on the continuum mechanics, developed by R. Hobart [R. Hobart (1965)], in order to describe the dynamics of dislocations in competing slip systems.

At that time an atomic picture of a dislocation, the Frenkel-Kontorova one, was already available: a chain of atoms, connected by interatomic harmonic springs, ready to slip, like a caterpillar, in a sinusoidal potential well modeling the rigid substrate of the non-dislocated ideal crystal. (Fig. 5) Hobart's model allowed to calculate the Peierls energies and the Peierls stresses of candidate slip systems for fcc and bcc metals. In practice these quantities represent the energy and the stress needed by a dislocation in order to climb from its stable to unstable equilibrium configuration. Notwithstanding the atomistic nature of the Frenkel-Kontorova picture of the dislocation, in order to calculate the above quantities, instead of using directly the relevant interplanar force constants, the model developed by R. Hobart utilized the Young modulus, the shear modulus and the Poisson ratio from continuum mechanics.

We modified the Hobart's values of to represent properly the 2D nature of the (unit length of) the glide dislocation line (for details see S. Boffi, G. Caglioti, G. Rizzi and F. Rossitto, 1973) (see Fig. 5). For the highly symmetric cubic structures, it was easy to attribute adequate weight, in the atomistic expressions of  $\alpha$  and  $\kappa$ , to the interplanar contributions not only of nearest neighbors, but also of higher order neighbors.

To a difference with respect to Hobart's findings, our approach to the description of the slip systems in terms of interplanar force constants could account for puzzling experimental facts, such as the easy (100)[011] slip system of

Nb: we attributed this anomalous behavior to the remarkable stiffness of the [100]L branch at low wavevectors, and to the exceptional softness, again at low wavevectors, of the [011]T branch polarized along the slip direction [0 $\bar{1}$ 1]. (For the dispersion curves of niobium see Y. Nakagawa and A. D. B. Woods (1963)).

Thereafter our calculations were extended to the Peierls energies and the Peierls stresses of candidate (1120)[1100] prismatic and (1120)[0001] basal slip systems for some hcp metals: in particular Zn, Mg, Ti and Zr [4]. However in applying our atomistic reformulation of the Hobart's model to the hcp structures, it was possible to include only first neighbor interplanar force constants. Our results are reported in Table 1 (taken from S. Boffi and G. Caglioti, 1973) and compared with those obtained by applying the Hobart model based on the continuum theory [5].

Basal slip is strongly preferred to prismatic slip for Zn: this metal, characterized by an axial ratio  $c/a = 1,85$  remarkably larger than the ideal one ( $= 1.633$ ), exhibits lower Peierls stresses and lower Peierls energies for the basal system than for the prismatic slip system, according both to the Hobart model based on continuum mechanics and to its atomistic version developed by us.

Prismatic slip is only slightly preferred to basal slip for Zr, and Ti, according again to both the Hobart model and its atomistic version.

As far as Mg is concerned, while the Hobart model indicates prismatic slip as the favored slip system, its atomistic version, though slightly, prefers basal slip to prismatic slip, in agreement with the behavior of the critical resolved shear stress reported by Couret and Caillard (1985). However the relative importance of the prismatic slip in this crystal is not negligible: Hiroshi Asada and Hideo Yoshinaga, in a Japanese paper of 1959 on "Nonbasal Slip and Twins of Magnesium", report an observation of the secondary nonbasal slip (10 $\bar{1}$ 0) [1 $\bar{2}$ 10] at high temperature.

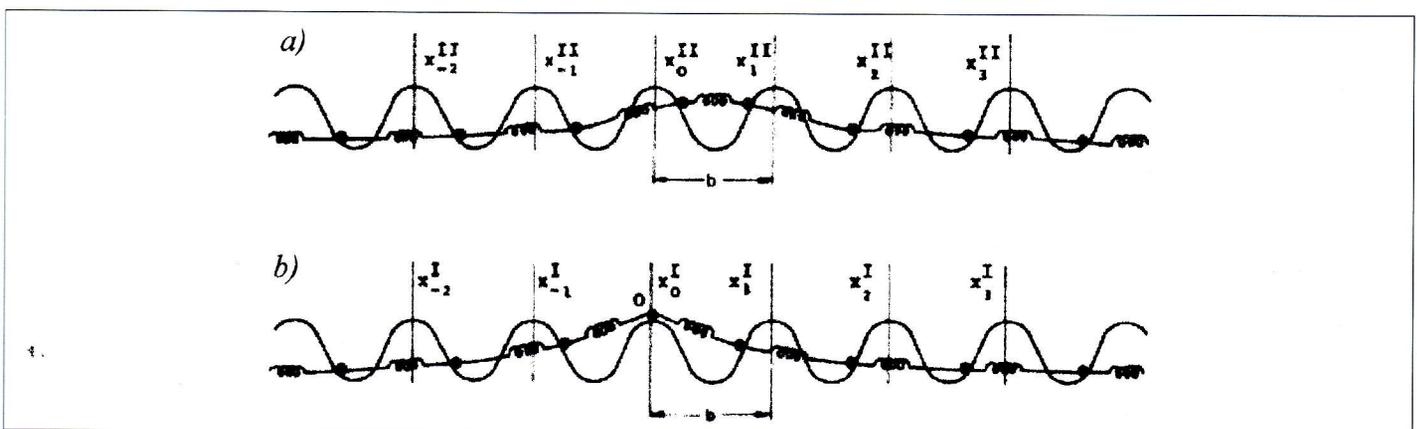


Figure 5: a) the stable and b) the unstable equilibrium configuration of a Frenkel-Kontorova edge dislocation of Burgers vector  $b$ . A row of  $N+1$  atoms above the slip plane, connected by harmonic springs of force constant  $\alpha$  between nearest neighbors, sits in the sinusoidal potential well of caliper amplitude and maximum curvature proportional to  $\kappa$ , with  $N$  minima schematizing the substrate of the 1D non-dislocated crystal. The equilibrium configurations are controlled, in practice, by the ratio  $\kappa/\alpha$ . In the Hobart model this ratio between interplanar force constants  $\kappa$  and  $\alpha$ , associated to transverse (T) and longitudinal (L) modes respectively, was expressed in terms of the shear modulus, the Young modulus and the Poisson ratio.

**TABLE 1 - Peierls Energy  $E_p$  (erg/cm) and Peierls stress  $\sigma_p$  (dyne/cm<sup>2</sup>) of some hcp metals, as computed within the frame of the lattice dynamics approach (columns A) and the continuum theory (columns B).**

Element	Glide system	A		B	
		$E_p$	$\sigma_p$	$E_p$	$\sigma_p$
Cd	(0001) $[\bar{1}1\bar{2}0]$	—	—	$1.6 \times 10^{-9}$	$5.8 \times 10^6$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	—	—	$4.5 \times 10^{-9}$	$1.6 \times 10^7$
Zn	(0001) $[\bar{1}1\bar{2}0]$	$3.5 \times 10^{-14}$	$1.5 \times 10^2$	$6.2 \times 10^{-9}$	$2.7 \times 10^7$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	$1.9 \times 10^{-10}$	$8.5 \times 10^5$	$1.3 \times 10^{-8}$	$5.9 \times 10^7$
Mg	(0001) $[\bar{1}1\bar{2}0]$	$2.4 \times 10^{-10}$	$7.2 \times 10^5$	$1.4 \times 10^{-8}$	$4.1 \times 10^7$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	$3.3 \times 10^{-10}$	$1.0 \times 10^6$	$7.0 \times 10^{-9}$	$2.1 \times 10^7$
Co	(0001) $[\bar{1}1\bar{2}0]$	—	—	$3.3 \times 10^{-8}$	$1.67 \times 10^8$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	—	—	$1.7 \times 10^{-8}$	$8.4 \times 10^7$
Ti	(0001) $[\bar{1}1\bar{2}0]$	$1.4 \times 10^{-9}$	$3.8 \times 10^6$	$3.7 \times 10^{-9}$	$9.7 \times 10^6$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	$3.2 \times 10^{-11}$	$8.4 \times 10^4$	$1.6 \times 10^{-9}$	$4.1 \times 10^6$
Zr	(0001) $[\bar{1}1\bar{2}0]$	$7.4 \times 10^{-11}$	$2.2 \times 10^5$	$2.5 \times 10^{-8}$	$7.5 \times 10^7$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	$6.1 \times 10^{-11}$	$1.8 \times 10^5$	$1.1 \times 10^{-8}$	$3.1 \times 10^7$
Be	(0001) $[\bar{1}1\bar{2}0]$	$1.0 \times 10^{-8}$	$6.1 \times 10^7$	$2.6 \times 10^{-7}$	$1.6 \times 10^9$
	(10 $\bar{1}0$ ) $[\bar{1}1\bar{2}0]$	$4.9 \times 10^{-9}$	$2.9 \times 10^7$	$1.2 \times 10^{-7}$	$7.0 \times 10^8$

Finally, in contradiction with the experimental observations, both the Hobart model and its atomistic version prefer prismatic slip to basal slip in Be.

Notwithstanding the discrepancy just denounced, concerning a crystal whose low axial ratio ( $c/a = 1.57$  for Be) should indeed prefer prismatic slip to basal slip, the approach to plasticity in terms of the dynamics of atoms in the crystal structure seems physically more sound and slightly more reliable than the previous approach based on the continuum theory.

The present approach to the plasticity of metallic hcp crystals in terms of their structure dynamics applies to slip systems characterized by high symmetry, and, if relevant dispersion relations are not known, cannot be exploited to assess the performance of other slip systems of lower symmetry whose occurrence might be of utmost importance for the mechanical formability of this metal. I refer e.g. to the sudden onset, at 220 °C, of the (1011)  $[\bar{1}2\bar{1}0]$  pyramidal slip,

observed in Mg by H.Asada and H.Yoshinaga in their paper on Temperature and Orientation Dependence of the Plasticity of Magnesium Single Crystals (in Japanese, 1959). I refer also e.g. to the a+c 1/3 (0111)  $[\bar{1}1\bar{2}3]$  pyramidal slip system carefully investigated by M. Koiwa in these proceedings [see also 6-8].

In order to explore the two slip systems above it would be necessary to measure phonon dispersion curves along reduced symmetry directions such as:

$[\bar{1}0\bar{1}1]T$  polarized along  $[\bar{1}2\bar{1}0]$  and  $[\bar{1}2\bar{1}0]L$ , related to the  $\kappa$  (transverse type) and  $\alpha$  (longitudinal type) of interplanar force constants respectively;  $[0\bar{1}11]T$  polarized along  $[\bar{1}1\bar{2}3]$  and  $[\bar{1}1\bar{2}3]L$ , related to the  $\kappa$  (transverse type) and  $\alpha$  (longitudinal type) of interplanar force constants respectively..

However, to my knowledge, these neutron spectroscopy experiments have not been undertaken yet.

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