Influence of Elastic Anisotropy on the Dislocation Contribution to the Elastic Constants*

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Calculations of the dislocation contribution to the measured elastic constants of face-centered cubic crystals are made as follows. First, the displacement of a pinned dislocation segment under an externally applied stress is evaluated. Then the contribution to the resulting macroscopic distortion of the specimen resulting from the motion of all the dislocations present is calculated. The results are that the contributions for given dislocation arrangements increase with increasing anisotropy. For copper and lead the contributions can amount to a few percent in a pure well annealed crystal and can be as large as 10% in slightly deformed crystals. Edge dislocations are found to make about ten times larger contributions than a similar density of screw dislocations.

I. INTRODUCTION

IT has been known for some time that the internal friction and the elastic constants of elastically anisotropic crystals even when measured at very low strain amplitudes are rather sensitive to the dislocation density. This paper attempts to calculate the dislocation contribution to the elastic constants and it attempts to describe how the dislocation and perfect crystal contributions to the elastic constants can be obtained experimentally. The calculations are given in a form suitable for the face-centered cubic metals, but the basic concepts can be applied to any crystal.

Eshelby[1] was the first to note that the presence of dislocations would lower the measured elastic constants. In 1952 a detailed calculation[2] of the motion under a small oscillating stress of a dislocation pinned down by impurity atoms was given. This calculation showed that the reversible dislocation motion gives rise to a small extra strain which is interpreted in elastic constant measurement to mean a smaller elastic constant than is actually appropriate for the perfect crystal. If the dislocations are very thoroughly pinned down by impurity atoms then this picture predicts that they will not make any appreciable contribution to the elastic constants. Recently Thompson and Holmes[3] have obtained beautiful data in which they have pinned down the dislocations in 99.999% pure copper single crystals. These data are given in Table I. Thompson and Holmes point out that the defect concentrations introduced by such irradiations are so small that it is inconceivable that the changes are a result of alterations of the perfect crystal elastic constants.

Two points should be noted. Marx and Koehler[4] and later Bradfield and Pursey[5] demonstrated that in copper single and polycrystals, respectively, small amounts of impurity can pin down the dislocations and hence increase the elastic constants. Less than one atomic percent of impurities is required. In addition, small amounts of cold work produce large changes in the measured elastic constants. Probably the large 9.55% change in Young's modulus observed by Thompson and Holmes in specimen 1*A* (see Table I) was the result of a small deformation. Another example concerns NaCl. Granato, de Klerk, and Truell[6] found that the velocity of compressional elastic waves along the (100) direction increased with frequency 0.5% from 1 to 100 megacycles per second in undeformed NaCl. After a 0.06% compression, a 4% increase was observed. They attribute the increase to the inability of the dislocations to follow the rapid oscillations.

II. THE NATURE OF THE DISLOCATION CONTRIBUTION

There are two kinds of problems which must be discussed to clarify the dislocation contribution to the elastic constants. First, how does each pinned down length of dislocation move in response to an external applied stress. Second, knowing how each loop behaves, what is the contribution of all the dislocations to the elastic constants. The first problem contains the major physical points involved. The second is essentially an

TABLE I. Increase in Young's modulus of copper single crystals produced by pile irradiation (data of Thompson and Holmes).

Crystal	$E_0(10^{12}$ dyne/cm$^2)$	E_f	$\frac{(E_f-E_0)}{E_0}$	Integrated flux (nvt)
1*A*	1.227	1.344	0.0955	15×10^{17}
2*A*	1.008	1.023	0.0149	10×10^{17}
2*B*	1.013	1.028	0.0148	3.1×10^{15}
2*C*	1.021	1.0325	0.0113	10×10^{17}
3*A*	1.460	1.472	0.0082	10×10^{17}
3*B*	1.474	1.477	0.0022	8.5×10^{15}
4*A*	1.107	1.149	0.0380	2.4×10^{14}
83*A*	1.142	1.196	0.0472	4.8×10^{18}

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[1] J. D. Eshelby, Proc. Roy. Soc. (London) **A197**, 396 (1949).
[2] J. S. Koehler, in *Imperfections in Nearly Perfect Crystals* (John Wiley & Sons, Inc., New York, 1952), p. 197.
[3] D. O. Thompson and D. K. Holmes, J. Appl. Phys. **27**, 713 (1956).
[4] J. Marx and J. S. Koehler, *Plastic Deformation of Crystalline Solids*, Office of Naval Research Pittsburgh Conference, p. 171, 1950 (unpublished).
[5] G. Bradfield and H. Pursey, Phil. Mag. **44**, 437 (1953).
[6] Granato, de Klerk, and Truell, Phys. Rev. **108**, 895 (1957).

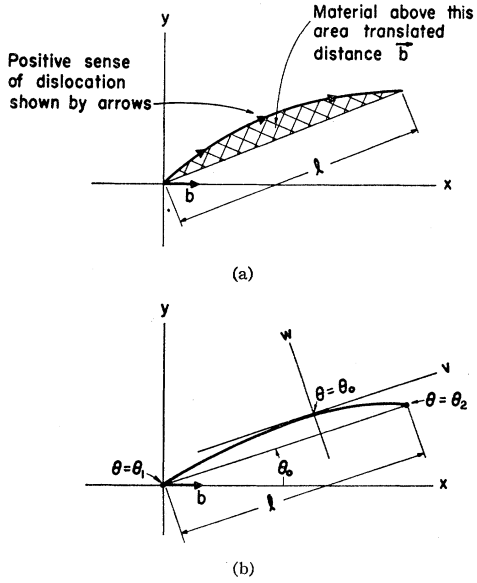

FIG. 1. (a) Quantities used to calculate change in strain due to dislocation motion. (b) Coordinate system used to calculate $\int dA$.

averaging problem. Let us consider the entire problem first.

To clarify the way in which a dislocation contributes to the total strain, it is useful to review an operational way of defining a dislocation:[7] make a cut in the material which ends on the dislocation line; choose the surface of the cut which would be reached first if the dislocation is encircled in the direction that a right hand screw turns in order to advance in the positive direction of the dislocation; translate this surface by **b** with respect to the other surface; glue the material together again and let it relax. When an external shearing stress is applied, a dislocation line pinned at its ends bows out. The material above the area swept out by the dislocation is translated by **b** relative to the material below this area. Let the xy plane be the slip plane; let x be in the direction of the Burger's vector. The resolved shearing stress is σ_{xz}. Suppose $\int dA\,(l,\theta_0,\sigma_{xz})$ is the area swept out by the dislocation as the stress increases from zero to its final value and $N(l,\theta_0)dld\theta_0$ is the total length of dislocations per unit volume which have lengths between l and $l+dl$, and whose Burger's vectors make angle between θ_0 and $\theta_0+d\theta_0$ with the dislocation in the unstressed condition (see Fig. 1, the curve x *versus* y represents the bowed out dislocation). Let $\epsilon_{xz}(l,\theta_0,\sigma_{xz})dld\theta_0$ be the average shearing strain caused by the motion of such dislocations. Note that the average shearing strain produced by the motion of each dislocation loop is:[8]

$$\frac{b}{2V}\int dA\,(l,\theta_0,\sigma_{xz}),$$

where V is the volume of the specimen. The number of loops of a specified type in V is $N(l,\theta_0)Vdld\theta_0/l$. Hence we find that the average shearing strain associated with the motion of these dislocations is:

$$\epsilon_{xz}(l,\theta_0,\sigma_{xz})dld\theta_0=(b/2l)N(l\theta_0)\int dA\,(l,\theta_0,\sigma_{xz})dld\theta_0. \quad (1)$$

The strain given by (1) is associated only with dislocations originally characterized by l, θ_0, and with one particular Burgers vector and occuring in slip planes of one orientation. To get the final macroscopic result the strain would have to be integrated over l and θ_0, and averaged over the area of the slip plane if $N(l,\theta_0)$ varies in space. Then the contributions from dislocations in various slip planes and with various Burgers vector (e.g., all the {111} planes and all the ⟨110⟩ directions in face-centered cubic crystals) would have to be combined. This could be done by choosing some axes fixed in the crystal and, by usual tensor methods, taking the components along these axes of the e_{xz} for each slip system, and adding. It should be mentioned that the σ_{xz} which occurs in $\int dA$ in (1) is also a function of the orientation of the slip planes, since it is some component of the stress applied to the crystal.

Evaluation of $\int dA$

The area swept out by the dislocation in reaching its equilibrium position must now be calculated. In an earlier paper an expression is obtained[9] which gives the shape of a dislocation in an elastically anisotropic crystal under an applied stress as the solution of the differential equation of equilibrium. It is found that one cannot, in general, get an explicit expression for the constants of integration such that the dislocation curve passes through the fixed end points, that is, to identify which part of the curve x *versus* y (the general solution to the differential equation) represents the dislocation. Thus $\int dA$ cannot be evaluated in general. However, if σ_{xz} is sufficiently small, an approximate relation for $\int dA$ can be obtained.

To calculate the area swept out by a dislocation segment which originally was of length l and made an angle of θ_0 with the Burgers vector, define a local coordinate system (v,w) with origin at the point on the curve x *versus* y where the tangent makes an angle of θ_0 with the Burgers vector, and with the v axis tangent to the curve at this point. See Fig. 1. Thus

$$\begin{aligned} v(\theta)&=[x(\theta)-x(\theta_0)]\cos\theta_0+[y(\theta)-y(\theta_0)]\sin\theta_0,\\ w(\theta)&=-[x(\theta)-x(\theta_0)]\sin\theta_0+[y(\theta)-y(\theta_0)]\cos\theta_0. \end{aligned} \quad (2)$$

Finally, $\int dA$ can be evaluated as

$$\int dA=\int_{\theta=\theta_1}^{\theta_2}[w(\theta)-w(\theta_1)]dv(\theta).$$

[7] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Oxford University Press, New York, 1953), p. 15.
[8] See reference 7, p. 19.
[9] G. deWit and J. S. Koehler, preceding paper [Phys. Rev. **116**, 1113 (1959)].

In the earlier paper it is shown that the shape of a dislocation lying in a glide plane under an external shearing stress σ_{xz} is given by:[9]

$$x=c_2-\{\sigma_{xz}b\}^{-1}\{\sin\theta E(\theta)+\cos\theta(dE/d\theta)\},$$
$$y=c_1+\{\sigma_{xz}b\}^{-1}\{\cos\theta E(\theta)-\sin\theta(dE/d\theta)\}, \quad (3)$$

where $E(\theta)$ is the energy required to produce unit length of dislocation having angle θ between the tangent to the dislocation and the Burgers vector. Dislocation interactions are neglected in Eq. (3). It will be assumed that the dislocation does not bow out much so that $\theta_1-\theta_0$ and $\theta_2-\theta_0$ are much less than one. We then insert x and y from (3) into (2) and expand about θ_0. One finds:

$$v(\theta_2)-v(\theta_1)=l, \quad w(\theta_2)-w(\theta_1)=0. \quad (4)$$

Finally $\int dA$ can be evaluated as:

$$\int dA=\int_{\theta_1}^{\theta_2}[w(\theta)-w(\theta_1)]dv(\theta). \quad (5)$$

If this procedure is carried out, the following is obtained

$$(\theta_1-\theta_0)=-(\theta_2-\theta_0)=\tfrac{1}{2}\epsilon,$$
$$v(\theta_2)=-v(\theta_1)=\tfrac{1}{2}l,$$
$$w(\theta_2)=w(\theta_1)=-\tfrac{1}{8}\epsilon l,$$
$$\int dA=\tfrac{1}{2}\epsilon l^2,$$

where

$$\epsilon=b\sigma_{xz}l/(E+d^2E/d\theta^2)_0. \quad (6)$$

In the above, $(\,)_0$ means that quantity in parentheses is evaluated at $\theta=\theta_0$. The quantity ϵ must be small if (6) is to be valid. The strain ϵ_{xz} can now be found from (1) as follows:

$$\epsilon_{xz}(l,\theta_0,\sigma_{xz})dld\theta_0=(1/24)N(l,\theta_0)bl\epsilon dld\theta_0. \quad (7)$$

If the preceding calculation is carried out to a higher order of approximation, ϵ_{xz} also has a term in ϵ^3.

The Integrating Process

As mentioned before, the strain given in (7) must be summed as follows:

$$\epsilon_{xz}=\int\int dld\theta_0\epsilon_{xz}(l,\theta_0,\sigma_{xz}), \quad (8)$$

where ϵ_{xz} is the total strain caused by the motion of all the dislocations in one slip system.

There is a possible difficulty associated with the evaluation of (8). In order for the expressions (7) and (8) to be valid, the following must be satisfied:

$$\epsilon=[b\sigma_{xz}l/(E+d^2E/d\theta^2)_0]\ll 1. \quad (9)$$

Thus σ_{xz} must be chosen so small that (9) is valid for the largest value of l which would be included in the integral (8). It would be hard to satisfy (9) if $(E+d^2E/d\theta^2)_0$ approaches zero, as it might in some cases.

TABLE II. Slip systems for the face-centered cubic crystals.

Unit normal to slip plane	Unit vector in direction of **b**
$3^{-\frac{1}{2}}(111)$	$2^{-\frac{1}{2}}(0\bar{1}1)$
	$2^{-\frac{1}{2}}(10\bar{1})$
	$2^{-\frac{1}{2}}(1\bar{1}0)$
$3^{-\frac{1}{2}}(\bar{1}11)$	$2^{-\frac{1}{2}}(01\bar{1})$
	$2^{-\frac{1}{2}}(101)$
	$2^{-\frac{1}{2}}(110)$
$3^{-\frac{1}{2}}(1\bar{1}1)$	$2^{-\frac{1}{2}}(011)$
	$2^{-\frac{1}{2}}(10\bar{1})$
	$2^{-\frac{1}{2}}(110)$
$3^{-\frac{1}{2}}(11\bar{1})$	$2^{-\frac{1}{2}}(011)$
	$2^{-\frac{1}{2}}(101)$
	$2^{-\frac{1}{2}}(1\bar{1}0)$

If it is assumed that σ_{xz} is small enough so that (9) is satisfied, then ϵ_{xz} takes the form

$$\epsilon_{xz}=(\sigma_{xz}/24)\int\int[dld\theta_0 \times N(l,\theta_0)b^2l^2/(E+d^2E/d\theta^2)_0]=S\sigma_{xz}. \quad (10)$$

If it is also assumed that $N(l,\theta_0)$ is independent of σ_{xz}, then S will also be independent of σ_{xz}. In deriving the equilibrium shape of the dislocation given by (3) σ_{xz} was taken to be constant. If an attempt is made to apply (10) to a case where σ_{xz} varies in space, but slowly enough so that it is essentially constant over the length of the dislocation segment, then the assumption that $N(l,\theta_0)$ is independent of σ_{xz} may be poor.

Geometric Aspects of the Problem

The last step in finding the dislocation contribution so the elastic moduli, that is, combining the effects due to dislocations in the various slip systems, will now be considered for the case of the face-centered cubic crystal. The procedure is as follows. Using the cubic axes of the crystal for reference, an arbitrary stress field σ_{ij} is assumed. The value of σ_{xz} for each slip system is found in terms of σ_{ij}. Using (10), the dislocation contribution to the strain ϵ_{xz} is obtained and its components with respect to the reference axes evaluated. It is assumed that S, in (10), is a constant and the same for all slip systems. When the contributions from all the slip systems are added, the result is $\delta\epsilon_{ij}$, the total dislocation contribution to the strain, referred to the cubic axes and expressed in terms of the applied stress.

The twelve slip systems are listed in Table II. The results of the calculation are

$$\delta\epsilon_{11}=(8/3)S\sigma_{11}-(4/3)S\sigma_{22}-(4/3)S\sigma_{33},$$
$$\delta\epsilon_{22}=-(4/3)S\sigma_{11}+(8/3)S\sigma_{22}-(4/3)S\sigma_{33},$$
$$\delta\epsilon_{33}=-(4/3)S\sigma_{11}-(4/3)S\sigma_{22}+(8/3)S\sigma_{33},$$
$$\delta\epsilon_{23}=(4/3)S\sigma_{23},$$
$$\delta\epsilon_{31}=(4/3)S\sigma_{31},$$
$$\delta\epsilon_{12}=(4/3)S\sigma_{12}.$$

For the cubic crystals, the relation between stress and strain is[10]

$$\epsilon_{11}=S_{11}\sigma_{11}+S_{12}\sigma_{22}+S_{12}\sigma_{33},$$
$$\epsilon_{22}=S_{12}\sigma_{11}+S_{11}\sigma_{22}+S_{12}\sigma_{33},$$
$$\epsilon_{33}=S_{12}\sigma_{11}+S_{12}\sigma_{22}+S_{11}\sigma_{33},$$
$$2\epsilon_{23}=S_{44}\sigma_{23},$$
$$2\epsilon_{31}=S_{44}\sigma_{31},$$
$$2\epsilon_{12}=S_{44}\sigma_{12},$$

and thus it can be seen that

$$\delta S_{11}=(8/3)S,$$
$$\delta S_{22}=-(4/3)S,$$
$$\delta S_{44}=(8/3)S,$$

where δS_{ij} is the apparent change in S_{ij} due to dislocations.

Numerical Estimate of S

It is desirable to try to get some rough estimate of the magnitude of S. From (1) and (10)

$$S=(1/6)\int\int dld\theta_0 N(l,\theta_0)\pi l^2/[\ln(R/r_0)][K+d^2K/d\theta^2]_0, \quad (11)$$

where $E=[b^2K(\theta)/4\pi]\ln(R/r_0)$, R is the average dislocation separation, and r_0 is the core radius of a dislocation. Two very simple forms of $N(l,\theta_0)$ will be considered

$$N_0(l,\theta_0)=\delta(l-\bar{l})\delta(\theta_0-0)N(\bar{l},0),$$

and

$$N_{\pi/2}(l,\theta_0)=\delta(l-\bar{l})\delta(\theta_0-\pi/2)N(\bar{l},\pi/2), \quad (12)$$

where $\delta(x)$ is the Dirac delta function and $N(\bar{l},0)$ and $N(\bar{l},\pi/2)$ represent the density of screw and of edge dislocations, respectively, which are associated with one slip system. Both of the above represent a situation where all the dislocation segments have the same length, $\bar{l}$. In the first case, all the dislocations are screw, while in the second, all the dislocations are edge. If the integration in (11) is performed, S becomes

$$S_0=(\pi/6)N(\bar{l},0)\bar{l}^2/[\ln(R/r_0)][K+d^2K/d\theta^2]_{\theta=0},$$
$$S_{\pi/2}=(\pi/6)N(\bar{l},\pi/2)\bar{l}^2/[\ln(R/r_0)][K+d^2K/d\theta^2]_{\theta=\pi/2}.$$

It might be expected that a correct value of S would fall between S_0 and $S_{\pi/2}$.

An attempt must now be made to obtain approximate values for the various quantities appearing in the relations for S_0 and $S_{\pi/2}$.

$N(\bar{l},0)$ represents the number of cm of dislocation per unit volume in one slip system for the simple case in which all the dislocations are screw, while $N(\bar{l},\pi/2)$ is the corresponding quantity for the case in which all the dislocations are edge. Both of these will be approximated by:

$$N(\bar{l},\ )\cong N/n, \quad (14)$$

where N is a value which falls within the range of values observed experimentally for the total number of centimeters of dislocation per cm^3 in a crystal, and n is the number of slip systems.

If the pinning points are mostly dislocation nodes, a reasonable approximation for $\bar{l}$ might be

$$\bar{l}\cong N^{-\frac{1}{2}}. \quad (15)$$

However, if point defects are introduced into the crystal, $\bar{l}$ could be decreased without changing N. In constrast, deformation of a crystal might introduce some additional dislocations of long length, and thus increase N without decreasing $\bar{l}$.

If R is taken as the average distance between dislocations, then the correct order of magnitude is obtained if

$$R\cong N^{-\frac{1}{2}}. \quad (16)$$

The radius of the core is usually taken to be something like the length of the Burgers vector. For this rough calculation the following is sufficiently accurate for both Pb and Cu

$$r_0=b=3\times10^{-8}\text{ cm}. \quad (17)$$

From the relations derived in the previous paper it is found that $(K+d^2K/d\theta^2)$ has the following values in dynes/cm^2

	$\theta=0$	$\theta=\pi/2$
Pb	3.02×10^{11}	0.549×10^{11}
Cu	12.3×10^{11}	1.24×10^{11}

If the approximations given by (14) through (17) are used, and if N is taken as 10^6 cm^{-2}, the values obtained for S in cm^2/dyne are

	S_0	$S_{\pi/2}$
Pb	0.01×10^{-12}	0.08×10^{-12}
Cu	0.003×10^{-12}	0.03×10^{-12}

Since the change in each of the s_{ij} is of the order of S, a comparison of the above with the s_{ij} will give an idea of how significant the dislocation contribution might be. The s_{ij} are,[11] in cm^2/dyne

	Cu	Pb
s_{11}	1.49×10^{-12}	9.39×10^{-12}
s_{12}	-0.625×10^{-12}	-4.30×10^{-12}
s_{44}	1.33×10^{-12}	6.95×10^{-12}

The preceding tables indicate that the dislocation contribution to the elastic moduli is about a few percent. However, care should be taken in interpreting these

[10] The s_{ij} are defined for a system where $\epsilon_i=\Sigma s_{ij}\sigma_j$. The relation between the two systems is as follows: $\epsilon_1=\epsilon_{11}$, $\epsilon_2=\epsilon_{22}$, $\epsilon_3=\epsilon_{33}$, $\epsilon_4=2\epsilon_{23}$, $\epsilon_5=2\epsilon_{31}$, $\epsilon_6=2\epsilon_{12}$; $s_1=s_{11}$, $s_2=s_{22}$, $s_3=s_{33}$, $s_4=s_{23}$, $s_5=s_{13}$, $s_6=s_{12}$. The ϵ_i are not components of a tensor. Further discussion of this can be found in J. F. Nye, *Physical Properties of Crystals* (Clarendon Press, Oxford, 1957), Chaps. V, VI, and VIII.

[11] Cu, D. Lazarus, Phys. Rev. **76**, 545 (1949); Pb, E. Goens and J. Weerts, Physik. Z. **37**, 321 (1936).

results because many simplyifying assumptions have been used to derive the expressions in (13) and evaluate them numerically. In particular, note that S_0 and $S_{\pi/2}$ differ by a factor of 5 or 10, which indicates that the angular distribution is important and should be considered more carefully. Also, it should be mentioned that even though the expressions found in the earlier paper may be a fairly good approximation to K, it does not follow that the result of a double differentiation will yield an equally good approximation to $d^2K/d\theta^2$.

Some data of Thompson and Holmes are shown in Table I. The Young's modulus (which would be the reciprocal of s_{11} if the specimen axis were along a cubic axis of the crystal) is measured before and after pile irradiation. The difference between these is interpreted as the dislocation contribution since by thoroughly pinning the dislocations, the irradiation reduces or eliminates the dislocation motion. The change is of the same order of magnitude as calculated above and in well annealed elastically anisotropic crystals can amount to a percent or two of the elastic constants.

In slightly deformed crystals (such as Thompson and Holmes specimen 1A) the change can amount to 10%. The fact that anisotropic crystals give large dislocation motion for small stresses is also of importance if one considers the dislocation damping, i.e., the internal friction associated with dislocation motion. One expects that for specimens of comparable purity and perfection the logarithmic decrement at low strain amplitudes increases as the elastic anisotropy increases. Although a quantitative comparison is difficult, the present data do indicate a trend of this kind.[12]

[12] A. Granato and K. Lucke, J. Appl. Phys. **27**, 791 (1956).

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Relative Measurement of the Photodetachment Cross Section for H^-

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The spectral dependence of the photodetachment cross section for the negative ion of atomic hydrogen has been measured in the range from 4000 A to 13 000 A with approximately 300-A resolution. Measurements were made with twenty-five band pass filters, each measurement taken relative to the value obtained with a control filter at 5280 A. A probable error of about 2% is attached to the relative value obtained for each filter. The results are in significant disagreement with available calculated cross sections.

WE have carried out a careful measurement of the wavelength dependence of the photon absorption cross section of the negative ion of atomic hydrogen. A direct interest in this cross section has arisen from the fact that solar emissivity is controlled by H^-, through bound-free and free-free transitions. A special theoretical interest arises from the fact that the process is a particular case of the quantum-mechanical three-body problem; a wavelength dependence measurement would be useful in checking the success of various theoretical approximation methods.

The H^- photodetachment reaction is

$$H^- + h\nu \rightarrow H + e, \tag{1}$$

and the cross section for this is

$$\sigma \propto \left| \int \psi_b^* D \psi_c d\tau \right|^2. \tag{2}$$

Here D is a dipole length operator, ψ_b is the wave function for the H^- ion, and ψ_c is the wave function describing an outgoing electron in the field of the residual H atom. Approximations to ψ_b have been developed from the Ritz variational principle of minimum energy, using wave functions with various modifications and as many as 24 adjustable parameters[1,2] to calculate the electron binding energy of H^-. These calculations have satisfactorily converged on 0.754 ev, although no accurate experimental check exists. Furthermore, Chandrasekhar[3] has shown that values obtained for the cross section from Eq. (2), or from velocity and acceleration forms derived from Eq. (2), are not very dependent on the number of variational parameters used, above about ten. We can then believe that the H^- ground-state wave functions are quite good; and that internal inconsistencies in values calculated from Eq. (2), and from the velocity and acceleration forms derived from Eq. (2), are due mainly to the limitations of the plane-wave and static central field approximations used for the continuum state, ψ_c. No calculation of the photodetachment cross section presently available goes beyond the static

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