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CONTRIBUTION OF RADIATION DAMAGE TO THE STUDY OF BASIC ATOMIC MOTION IN SOLIDS

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Abstract

Radiation damage is a powerful tool for the study of point defect interactions in solids. The large numbers of point defects produced during irradiation and subsequent annealing aggregate to form planar and linear defects. A study of the nature of these defects provides basic understanding of the mechanics of defect formation in solids.

Defects in ion-bombarded silicon are studied using the transmission electron microscope. A mechanism for the formation of the observed defects is proposed. The utility of radiation damage studies in the understanding of atom motion in solids is demonstrated.

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I. INTRODUCTION

Radiation damage results from the deposition of the energy of the incoming radiation into the material irradiated. The irradiated material is transformed from a low to a high energy state. A part of the added energy appears as "radiation damage", or atoms displaced from their normal sites. In crystals, radiation damage results in the production of a large number of point defects (interstitials: atoms displaced from their normal sites and vacancies: empty lattice sites). In silicon, large areas in the region where the incoming particles come to a stop, are driven amorphous.

On annealing, the damage is repaired and the crystal reverts to a lower energy state. This occurs by point defects collecting into various types of clusters: stacking faults bounded by Frank dislocation loops and perfect prismatic dislocation loops are two important types. In this paper, defects produced on the annealing of ion damage in silicon are studied using the transmission electron microscope. Such studies suggest that certain families of the defects are absent. Their absence must therefore be intimately connected with the internal stresses resulting from radiation damage. A model in which the compressive stresses in the damaged regions aid the nucleation and growth of only those varients experimentally observed is proposed. An attempt is made to show that radiation damage studies are helpful in the understanding of basic atomic motion in solids.

II. EXPERIMENTAL

Samples of (111) silicon (0.5Ω cm p type) were bombarded with a high energy (100 kV) beam of phosphorous ions. The damaged samples were annealed in an inert stmosphere by heating to 800°C for 15-20 minutes. Samples for electron microscopy were chemically thinned and were examined in a Hitachi HU125 electron microscope.

III. ELECTRON MICROSCOPE RESULTS AND DEFINITION OF THE PROBLEM

The results, typical of the electron microscope observations, are shown in the bright field image (Fig. 1), the dark field image (Fig. 2) and the weak beam dark field image (Fig. 3) of the same area. The weak beam technique is a non-conventional imaging technique whereby very narrow images are obtained, as is clearly shown in Fig. 3. It is concluded from analysis of such pictures (Bicknell and Allen, Seshan, Bell and Washburn), that the small (500Å) hexagonal shaped loops are interstitial and have Burgers vector of the type $\frac{a}{2}\langle 110 \rangle$. Interstitial loops are formed by interstitials coalescing (Fig. 5). Vacancy loops are formed by the partial removal of an atomic layer by the congregation of vacancies.

The nucleation problem that needs to be explained may be defined with reference to the Thomson tetrahedron in Fig. 4. Prismatic dislocation loops have Burgers vectors $\frac{a}{2}\langle 110 \rangle$ lying along the six sides AB, BC, etc. of the Thomson tetrahedron. Frank loops have Burgers vector $\frac{a}{3}\langle 111 \rangle$ along Aα i.e., from an apex to the center of the opposite face.

In the most general case, therefore, prismatic loops with six possible $\frac{a}{2}\langle 110\rangle$ type Burgers vectors ought to be seen. Electron microscope studies show that only three are present in large numbers: these are along DA, DB and DC i.e., along $\langle 110\rangle$ directions inclined to the foil surface δ.

A mechanism for the formation of these loops must therefore explain

i. why there is a predominance of interstitial type loops.

ii. why most loops have Burgers vector inclined along $\langle 110\rangle$ directions.

IV. PROPOSED MODEL

i. Explaining the predominance of interstitial type loops.

Interstitial loops are formed by the collection and continuous addition of interstitials during annealing. The problem, therefore, consists in identifying the sinks for interstitials and vacancies during the annealing process.

It is known from experimental and theoretical work[3] that for light ions (P in this case) intense radiation damage is localized to the region where the bombarding radiation is brought to a halt. This results in a buried amorphous layer (BAL) at a depth of 500Å to 2000Å from the surface. It is further known that the volume of amorphous silicon is ~10% greater than the crystalline material.

The state of the material after irradiation is shown in Fig. 5. The BAL, being of greater volume than the surrounding crystalline material, expands. It is constrained in the direction parallel to the surface by the crystalline material around it. This sets up biaxial compressive stresses in the damaged material.

During annealing crystallinity is restored in the damaged regions accompanied by the clustering of the point defects to produce Frank loops. Nucleation and growth of that kind of Frank loop is most favored that most rapidly relieves the internal stresses due to damage. From the expected stress fields around the point defects in Fig. 5, it is clear that interstitials are attracted to the regions of tension just above and just below the damaged layer. Clustering of these interstitials results in interstitial Frank loops on the inclined {111} planes. The flux of interstitials from the damaged zone into the regions of tension is probably so high that predominantly interstitial loops are nucleated.

This model also predicts few vacancy type Frank loops to form parallel to the foil surface in regions of tension. The presence of such loops has recently been reported by Bicknell.[4]

ii. Explanation of the presence of only three of the six possible Burgers vectors.

The model proposed here is based on consideration of the atom motions required to unfault an $\frac{a}{3}\langle 111\rangle$ type extrinsic Frank loop.

Growth of the observed loops probably proceeds as follows: Isolated interstitials first reduce their energy by clustering on a (111) type close packed plane creating a planar defect or an extrinsic Frank loop with Burgers vector $\frac{a}{3}[111]$ e.g. Dδ in Fig. 4. At some critical size, the enclosed stacking fault is eliminated and a lower energy defect in produced by the unfaulting of the Frank loop to produce an $\frac{a}{2}\langle 110\rangle$ type prismatic loop. This occurs by the nucleation of a Shockley partial which sweeps away the stacking fault. The unfaulting sequence for an

$\frac{a}{3}$ [111] Frank loop lying on the δ plane is shown in Fig. 4.

Crystal structure require that only certain specific atomic motions cause the unfaulting of an extrinsic Frank loop. These atom motions are described in Figs. 6 and 7. In Fig. 6, the arrangements of atoms in a fcc metal is shown. In Fig. 7, the same atoms are viewed along the [111] body diagonal. There are certain restrictions on atom motion arising from the fact that it is energetrically unfavorable to bring two atoms in adjacent layers on top of each other. The allowed atom motions are shown in Fig. 7.

The unfaulting of a Frank loop probably proceeds by passage of two Shockley partials on successive layers. The resultant is a single Shockley partials such as δC, δB and δA on the δ plane in Fig. 4. On the inclined plane e.g. α these are αD, αB and αC.

The absence of the three $\frac{a}{2}\langle 110\rangle$ Burgers vectors AB, AC and BC may be explained with reference to Fig. 8a and b. Here (Fig. 8b) the Thomson tetrahedson in a state of biaxial compression. Such compression arises from the stress field of the interstitial Frank loops formed on the inclined planes (Fig. 8a). Reference to Fig. 8b shows that compression aids the motion of the three Shockleys αD, γD and BD. These three react with respective Frank Burgers vectors to produce to experimentally observed $\frac{a}{2}\langle 110\rangle$ inclined Burgers vectors.

In Fig. 9 is shown the effect of tension stress on loops lying on inclined planes. It is seen that in the presence of a biaxial tension stress interstitial loops form on inclined planes and vacancy loops on planes parallel to the (111) foil plane. Further, the stress has a zero-resolved shear stress on the planes parallel to the foil plane

(Schmidt Law) and does not aid the motion of Shockley partials. Therefore, according to this model, unfaulted Frank loops are expected on the (111) planes parallel to the foil.

It is of interest to note that precisely this observation has been made, experimentally, by R. W. Bicknell.[5]

V. CONCLUSION

Electron microscope studies of ion damaged silicon shows a predominance of extrinsic prismatic loops with only three of the six possible Burgers vectors. A model in which the compressive stresses produced by radiation damage may aid the formation and growth of such loops is proposed. It is shown that this model explains why a large number of the loops are interstitial and should have only those $\frac{a}{2}\langle 110\rangle$ Burgers vectors inclined to the foil surface. The importance of radiation damage to the understanding of basic processes in crystals is therefore demonstrated.

ACKNOWLEDGEMENTS

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2. K. Seshan, W. L. Bell and J. Washburn, Physica Status Solidi (A) (1971), to be published.

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5. R. W. Bicknell, private communication, J. of Microscopy, to be published.

FIGURE CAPTIONS

Fig. 1,2,3 Bright-field, dark-field and weak beam dark-field images of the same area. The tremendous reduction of image width using the weak-beam method is shown in Fig. 3. Analysis of such images show that the small hexagonal loops (500Å) are extrinsic and have Burgers vectors of the type $\frac{a}{2}\langle 100\rangle$ inclined to the (111) foil surface.

Fig. 4 The Thomson tetrahedron showing the arrangement of (111) planes in a fcc cell. The edges of the tetrahedron are made up of $\frac{a}{2}\langle 110\rangle$ type directions and are the Burgers vectors of prismatic dislocation loops. Frank loops have Burgers vectors from an apex to the center of the opposite face e.g. $D\delta$. The unfaulting sequence of a Frank loop with Burgers vector $D\delta$ is shown.

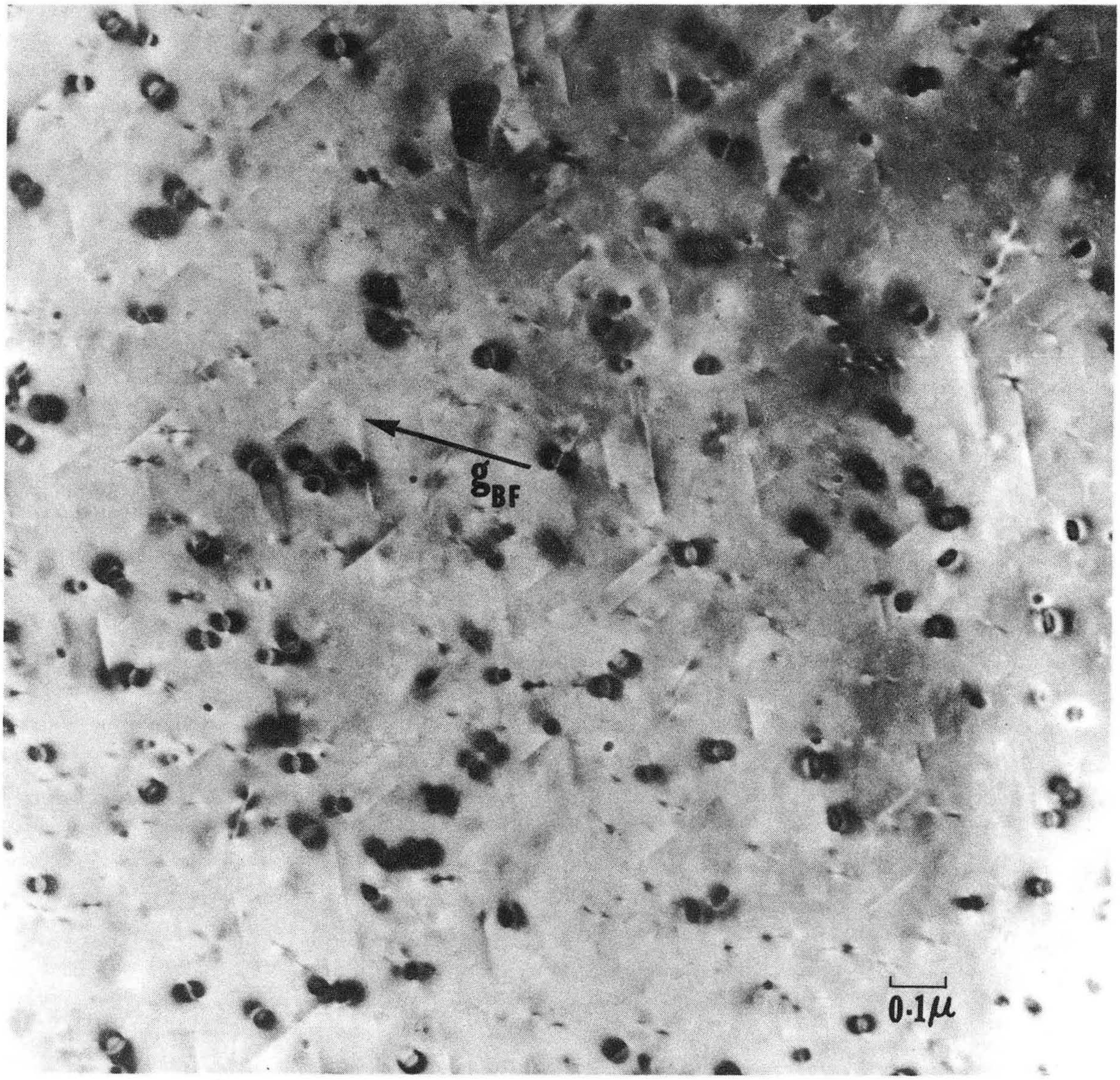
Fig. 5 The internal stresses caused by the radiation induced buried amorphous layer is shown. The amorphous material being of larger volume than crystalline material expands. Constrained by the surrounding crystalline material, compressive stresses are set up inside the damaged layer.

Fig. 6 and 7 The arrangement of atoms in an fcc crystal is shown. Figure 7 shows the cube viewed along the body diagonal. Any atom motion that brings two atoms on top of each other are energetically unfavorable. The resulting restrictions on the motion of atoms are shown in Fig. 7.

Fig. 8a Stress fields around the point defects show that interstitials collecting to form extrinsic Frank loops produce compressive stresses. This therefore helps explain why the loops which grow in the damaged region are extrinsic in nature.

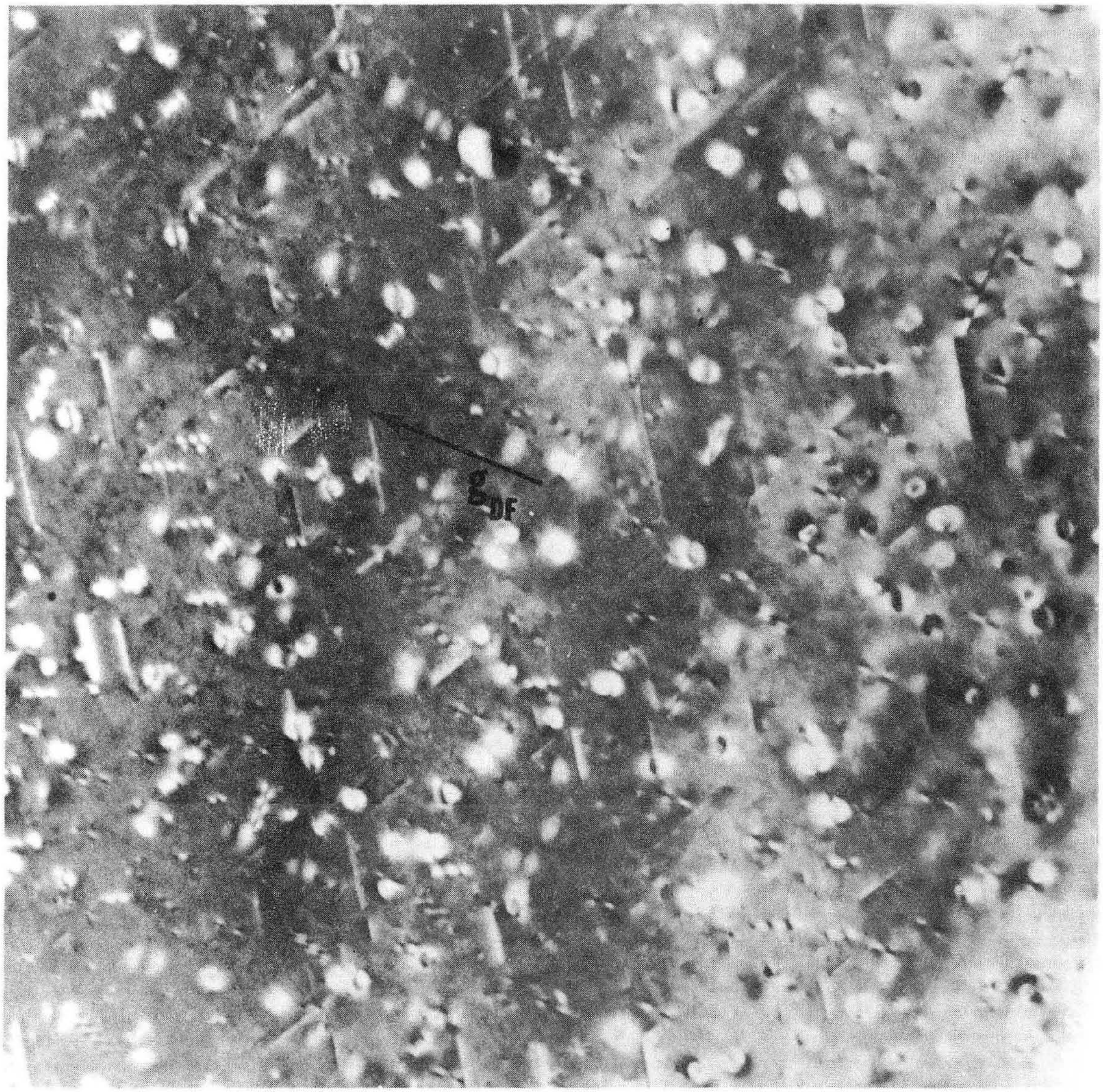
Fig. 8b The Thomson tetrahedron in a state of biaxial compression. Compressive stresses arise from the strain fields of the F interstitial Frank loops on the inclined planes. Compression aids the motion of the shockleys, αD, γD and BD only. The results are the predominance of the three $\frac{a}{2}\langle 110\rangle$ Burgers vectors AD, BD and CD found experimentally.

Fig. 9. Here the effect of a biaxial tension on the type of loops formed on the various (111) planes is illustrated. Such biaxial tension exists on either side of the damaged region as shown in Fig. 5. The biaxial tension favours the formation of vacancy loops on the (111) planes parallel to the foil surface and interstitial loops on the (111) planes inclined to the foil. Also note the resolved shear-stress in the foil plane is zero. So, no Shockley motion is expected. Therefore, unfaulted Frank loops may be expected on planes parallel to the foil. This is the experimental observation (Bicknell[5]).



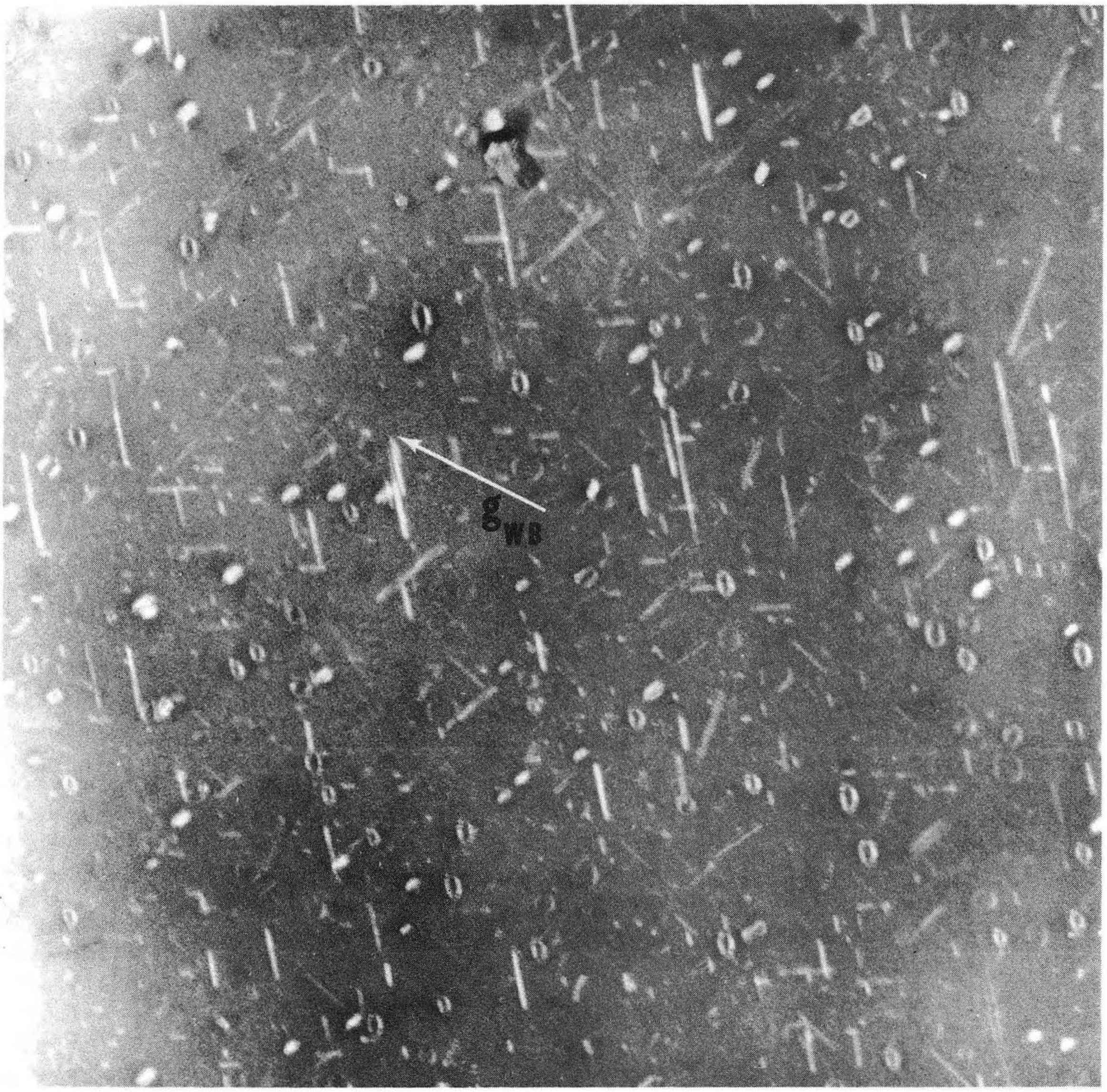
XBB 731-126

Fig. 1



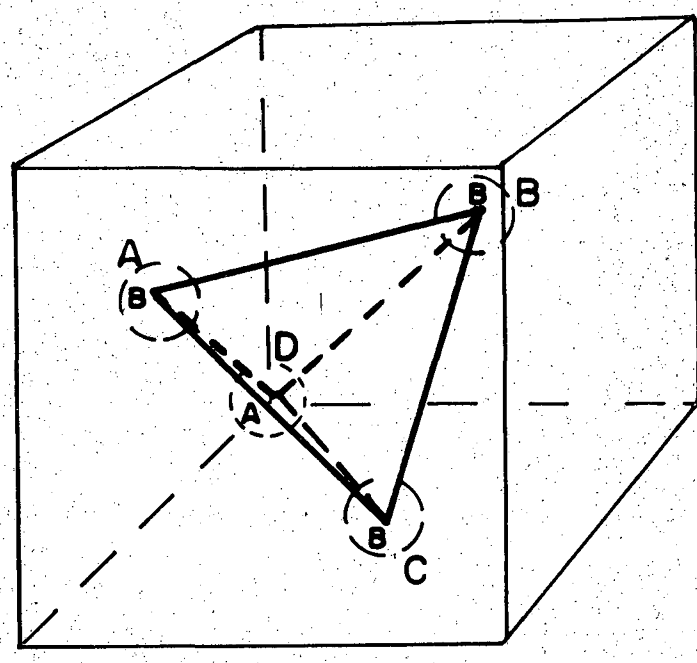
XBB 731-124

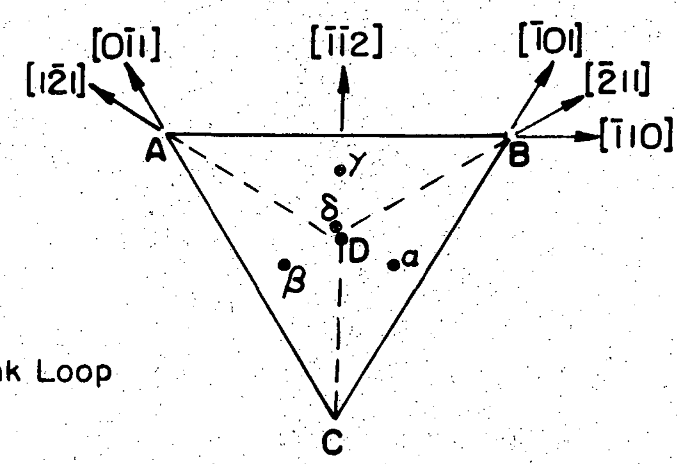
Fig. 2



XBB 731-125

Fig. 3





Unfaulting of Extrinsic Frank Loop

$$D\delta + \delta C = DC$$

$$\frac{a}{3}[111] + \frac{a}{6}[11\bar{2}] = \frac{a}{2}[110]$$

XBL 731-5635

Fig. 4

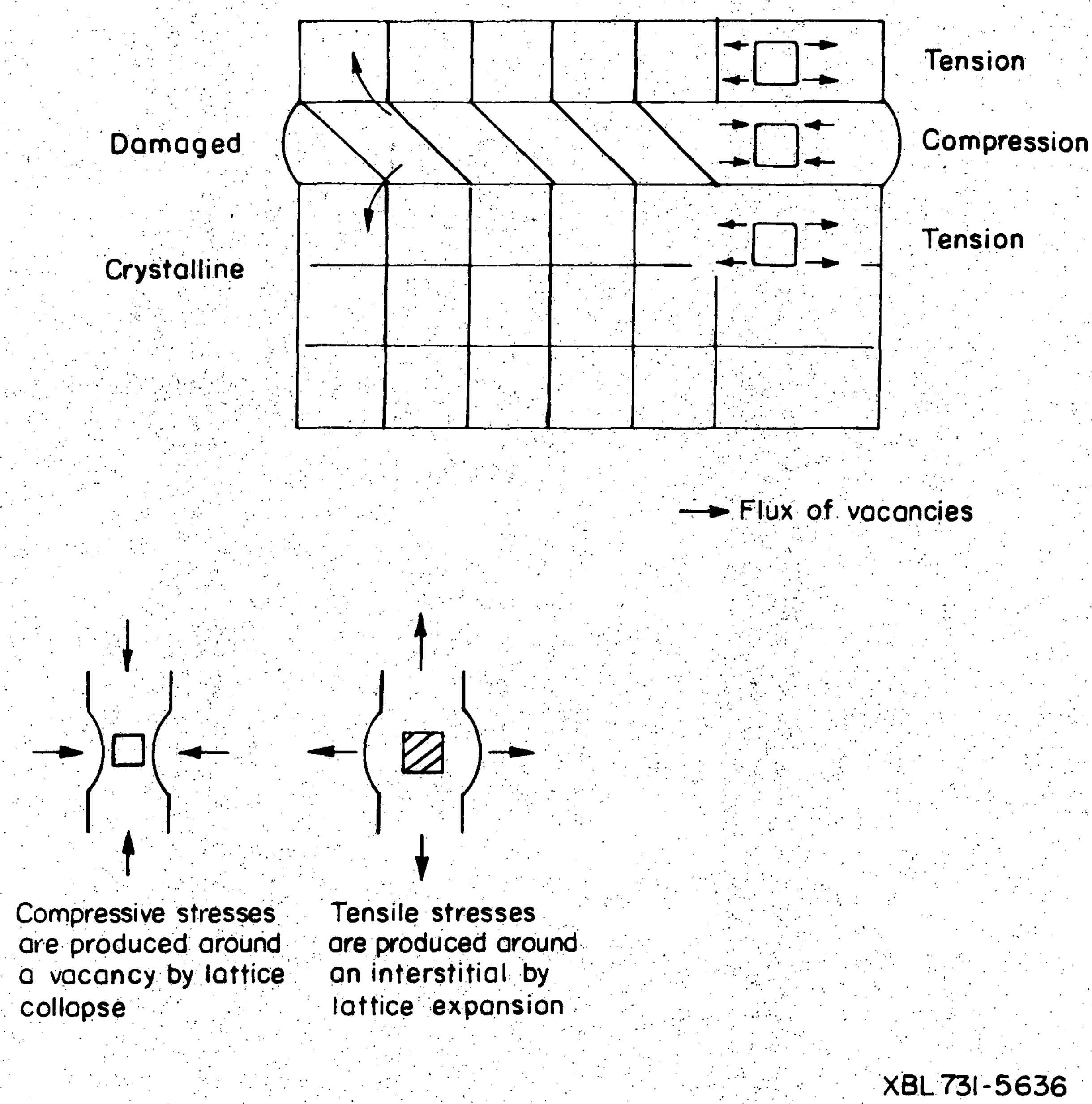
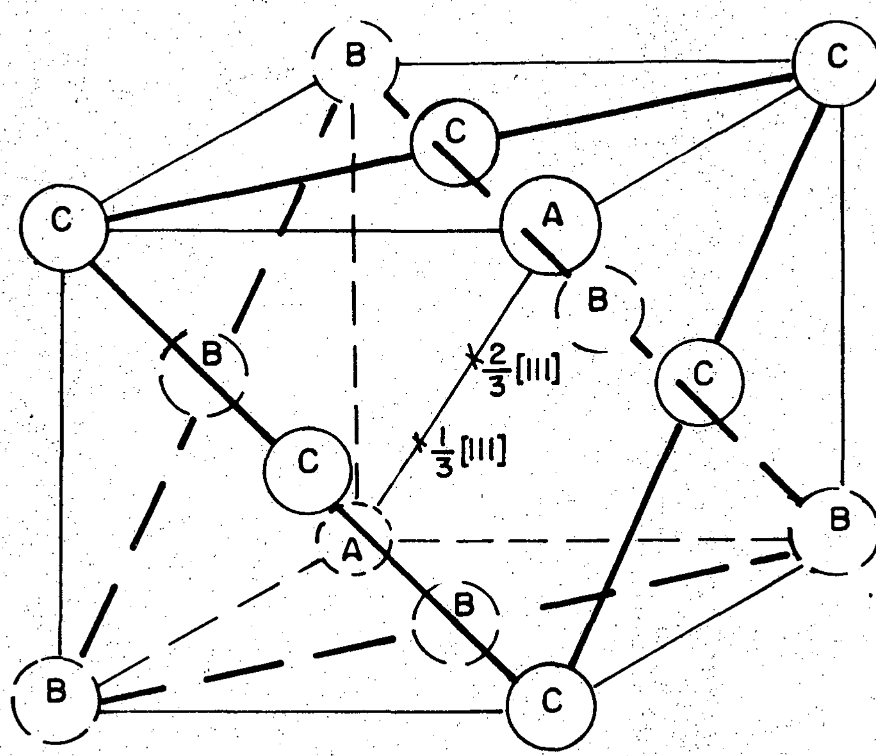
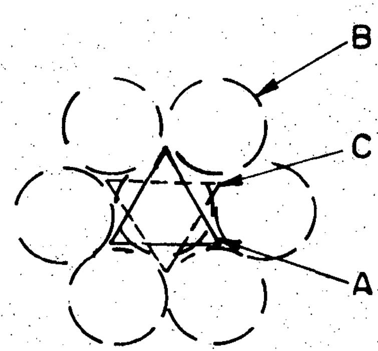

Tension
Compression
Tension
Damaged
Crystalline
Flux of vacancies
Compressive stresses are produced around a vacancy by lattice collapse
Tensile stresses are produced around an interstitial by lattice expansion
XBL 731-5636

Fig. 5





XBL731-5633

Fig. 6

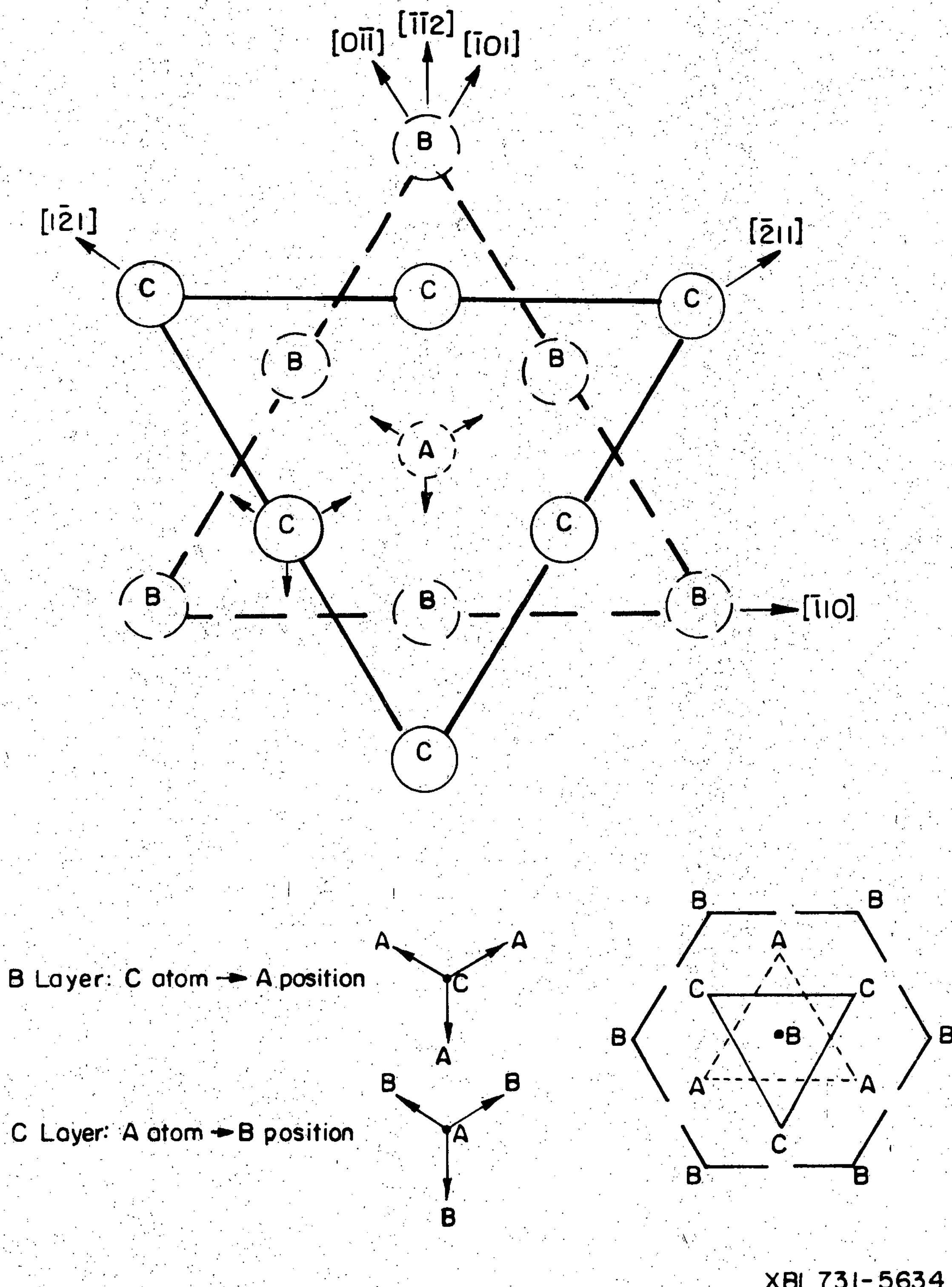

[0$\bar{1}\bar{1}$]
[$\bar{1}\bar{1}$2]
[$\bar{1}$01]
[1$\bar{2}$1]
[$\bar{2}$11]
[$\bar{1}$10]
B Layer: C atom → A position
C Layer: A atom → B position
XBL 731-5634

Fig. 7

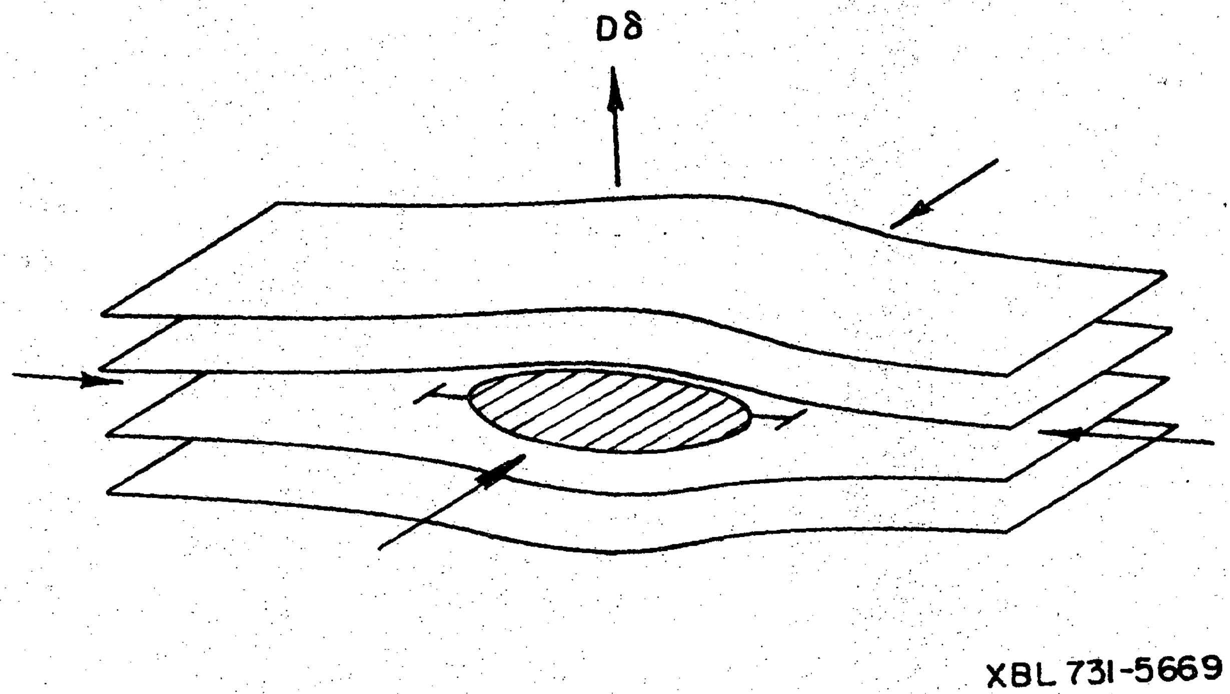
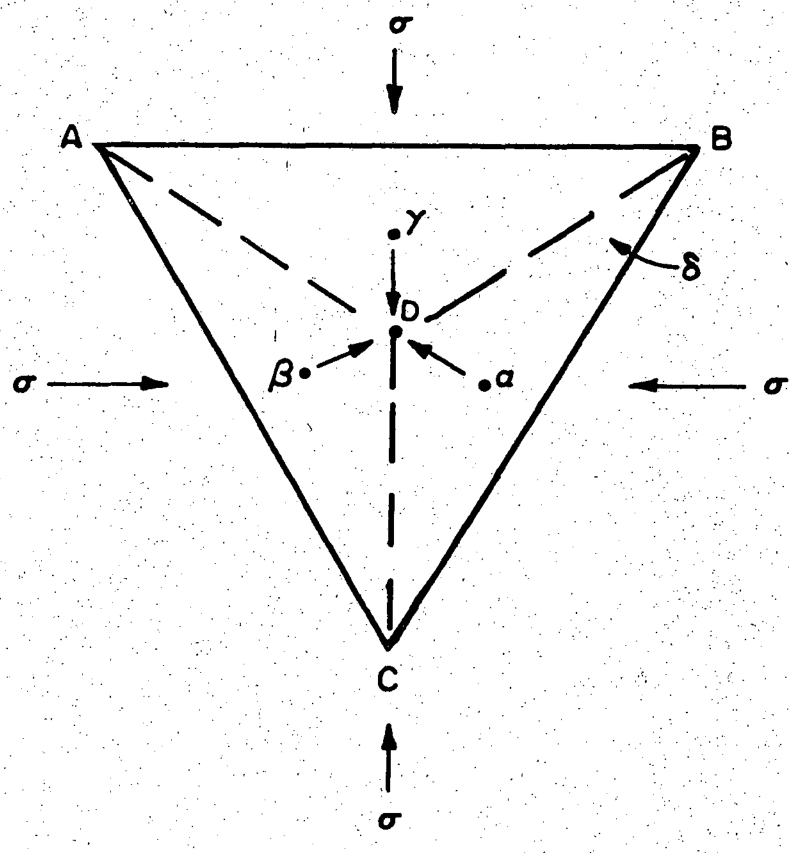


Fig. 8a



Interstitial Unfaulting

	Extrinsic Frank Loops		Shockleys		Extrinsic $\frac{a}{2}\langle 110\rangle$ Loops
δ plane	Dδ	+	δC	=	DC
	$\frac{a}{3}[1\bar{1}1]$	+	$\frac{a}{6}[11\bar{2}]$	=	$\frac{a}{2}[110]$
α plane	Aα	+	αD	=	AD
β plane	Bβ	+	βD	=	BD
γ plane	Cγ	+	γD	=	CD

XBL 731-5637

Fig. 8b

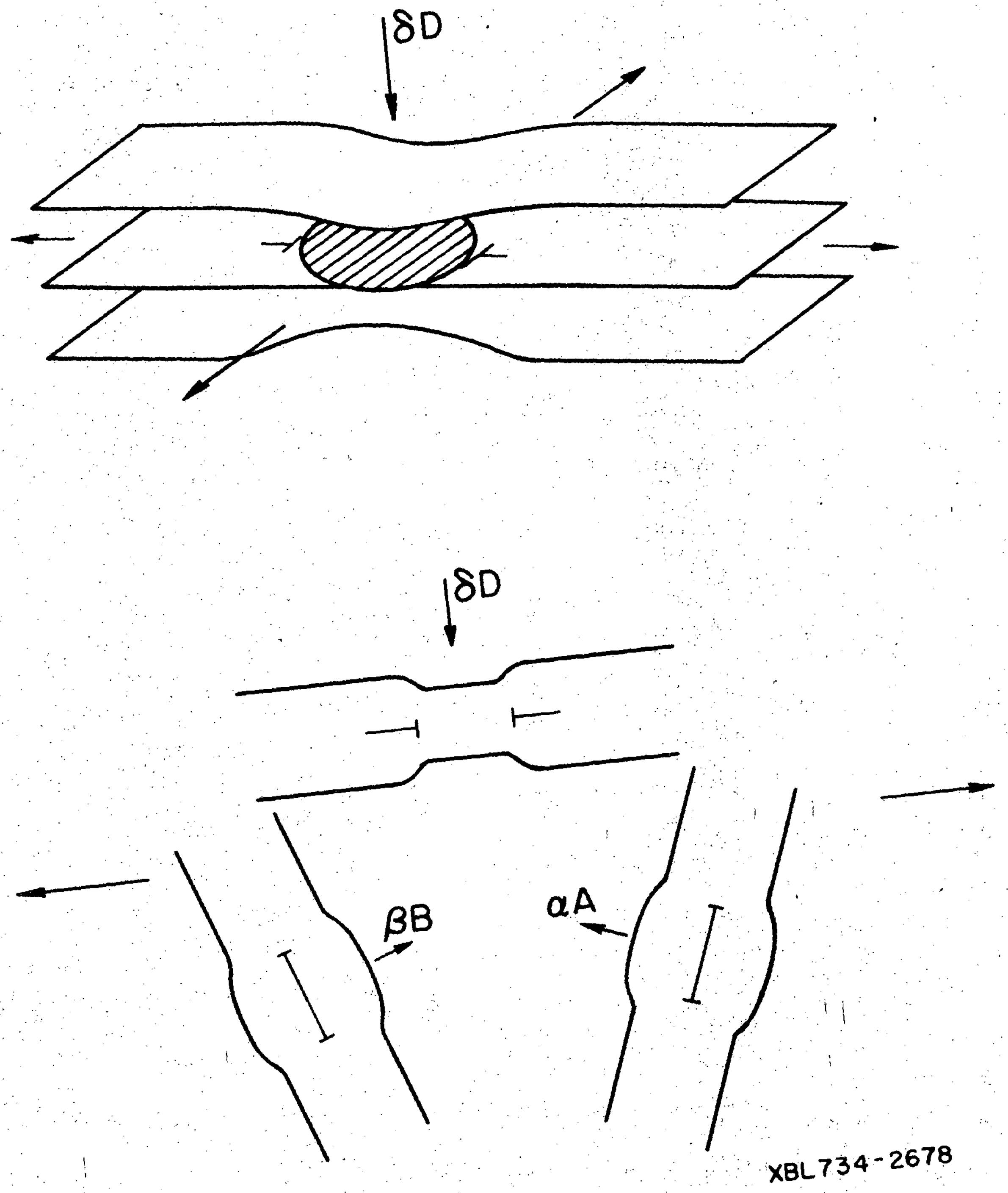


Fig. 9

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