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Effect of crystal structures on deformation behaviour of materials using finite element method

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ABSTRACT

This study presents the deformation analysis of crystalline materials considering three crystal structures viz. Fe (BCC), Co(HCP) and Ni(FCC). Deformation behaviour of these materials are modeled and analyzed using Finite Element Method considering identical billet upsetting on Abaqus software. The billet has been meshed with CAX4RT Elements. In this study both isotropic and anisotropic material properties have been considered. It is observed that anisotropy has dominant effect on FCC and BCC structures as compared to HCP.

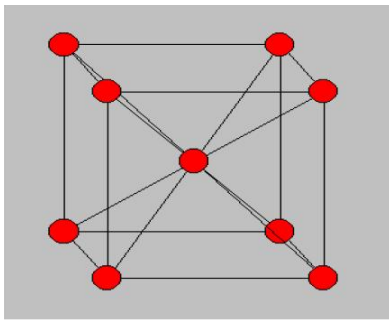
KEYWORDS

Deformation;
Upsetting;
Crystal;
Anisotropy.

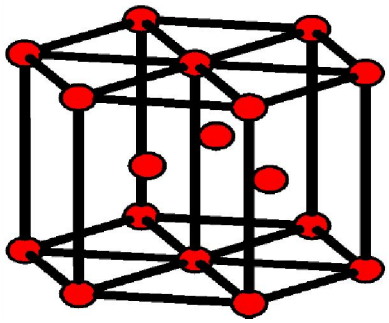
INRODUCTION

Crystal structure has direct bearing on the deformation behaviour of metallic materials[5]. The three most common crystal structures are Body centered cubic (BCC), Hexagonal close packed (HCP) and Face centered cubic (FCC) (Figure 1). Axiomatic properties which are considerably influenced by crystal structures are ductility, anisotropy etc. These properties directly influence the deformation processing of these materials. Some of the recent work dealing with material anisotropy and reported in literature are as follows:

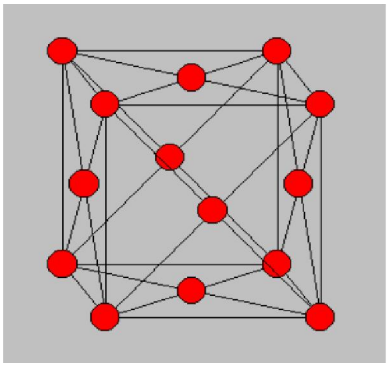
[1] proposed a method to study large deformation Finite Element simulations of anisotropic material using an updated Lagrangian finite element method[2] proposed a method in which combined finite element method-analytical approach has been used to study the elastic interaction of an axisymmetrical loaded ring plate with transversely isotropic medium. Two cases of transversely isotropic medium has been considered viz. homogenous isotropic halfspace and multilayer transversely isotropic halfspace[4] proposed a method to study thermomechanical simulation and processing of steel, in which they developed a scheme for integrating grain growth model in phase transition and grain distortion calculation in plastic deformation, which enables the simulation of microstructure evolution in steel processing when phase transition takes place during rolling[6]. proposed a method to study three-dimensional finite element simulations of microstructurally small fatigue crack growth in 7075 aluminium alloy[9] proposed a simulation study on fluctuant flow stress scale effect in which the crystal plasticity theory was used to simulate upsetting tests of different dimensions and grain size micro copper cylinders. Results showed that decrease of billet grain quantity, flow stress fluctuation is not always increased[10] proposed a method to study identification of elastic parameters of transversely isotropic thin films



(a) BCC Structure



(b) HCP Structure



(c) FCC Structure

Figure 1: (a) BCC Structure (b) HCP Structure (c) FCC Structure

by combining nanoidentation and FEM analysis. In this study the forward analysis CAX4R and CAX4E elements types of Abaqus are used to stimulate the purely mechanical indentation and piezoelectric indentation with assistance of substrate effect. The results show the transverse and longitudinal young modulus and the longitudinal shear modulus under the piezoelectric indentation mode are closer to the experimental values measured by the acoustic method than those under the purely mechanical indentation mode.

In this study linear elastic finite element simulation of three crystal structures viz. Fe(BCC), Co(HCP) and Ni(FCC) are carried out for identical upsetting deformation. Both isotropic and anisotropic material properties have been considered. Based on simulation results effects of anisotropic parameters of these crystal structures are critically examined in terms of stresses and load requirement.

MODELING PARAMTERS

In this study cylindrical billets made up of three crystal structures viz. BCC, HCP and FCC, are identically deformed and linear Finite element analyses are carried out considering isotropic and anisotropic material properties. Following modeling parameters are used for the analysis purpose:

(A). Geometricalparameters

The shape of the billets used for upsetting is cylindrical and the geometrical parameters are:
Height =0.50 m.
Diameter=0.15 m.

(B). Fe modeling

Billets are modeled and analysed using Abaqus Software. They are meshed with CAX4RT elements (4 nodes axisymmetric elements with reduced hourglass control). Because of symmetricity, axisymmetric modeling has been carried out. The number of elements are 1197 and the number of nodes are 1280. Finite Element Model is shown in Figure 2. Bottom nodes are free in X and fixed in Y directions whereas left side nodes are fixed in X and free in Y directions. A rigid punch is used to deform the billet. All the billets are identically deformed to 1 mm displacement.

(C). Material parameters:

Billet materials considered are Iron, Cobalt and

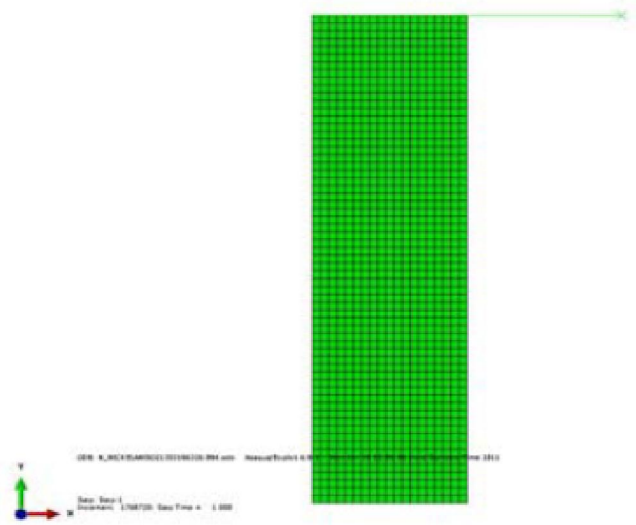


Figure 2 : FE Model

Nickel because they have different crystal structure such as body centered cubic, hexagonal closed packed and face centered cubic respectively. Both isotropic and anisotropic properties have been considered for each material.

The simplest form of linear elasticity is the isotropic case, and the stress-strain relationship is given by

$$\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{12}\\ \gamma_{13}\\ \gamma_{23}\end{Bmatrix} = \begin{bmatrix} 1/E & -\nu/E & -\nu/E & 0 & 0 & 0\\ -\nu/E & 1/E & -\nu/E & 0 & 0 & 0\\ -\nu/E & -\nu/E & 1/E & 0 & 0 & 0\\ 0 & 0 & 0 & 1/G & 0 & 0\\ 0 & 0 & 0 & 0 & 1/G & 0\\ 0 & 0 & 0 & 0 & 0 & 1/G \end{bmatrix} \begin{Bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{12}\\ \sigma_{13}\\ \sigma_{23}\end{Bmatrix}$$

The elastic properties are completely defined by giving the Young's modulus, *E*, and the Poisson's ratio, ν. The shear modulus, *G*, can be expressed in terms of *E* and as $G = E/2(1+\nu)$.

For anisotropic modeling Iron and Nickel are modeled as orthotropic anisotropy. Linear elasticity in an orthotropic material can be defined by giving the nine independent elastic stiffness parameters, the stress-strain relations are of the form-

$$\begin{Bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{12}\\ \sigma_{13}\\ \sigma_{23}\end{Bmatrix} = \begin{bmatrix} D_{1111} & D_{1122} & D_{1133} & 0 & 0 & 0\\ & D_{2222} & D_{2233} & 0 & 0 & 0\\ & & D_{3333} & 0 & 0 & 0\\ & & & D_{1212} & 0 & 0\\ & sym & & & D_{1313} & 0\\ & & & & & D_{2323} \end{bmatrix} \begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{12}\\ \gamma_{13}\\ \gamma_{23}\end{Bmatrix} = [D^{el}] \begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{12}\\ \gamma_{13}\\ \gamma_{23}\end{Bmatrix}$$

Cobalt is modeled as transverse anisotropic material. A special subclass of orthotropy is transverse isotropy, which is characterized by a plane of isotropy at every point in the material. Assuming the 1–2 plane to be the plane of isotropy at every point, transverse isotropy requires that $E_1 = E_2 = E_p$, $\nu_{31} = \nu_{32} = \nu_{tp}$, $\nu_{13} = \nu_{23} = \nu_{pt}$, and $G_{13} = G_{23} = G_t$, where *p* and *t* stand for "in-plane" and "transverse," respectively. Thus, while ν_{tp} has the physical interpretation of the Poisson's ratio that characterizes the strain in the plane of isotropy resulting from stress normal to it, ν_{pt} characterizes the transverse strain in the direction normal to the plane of isotropy resulting from stress in the plane of isotropy. In general, the quantities and are not equal and are related by $\nu_{tp}/E_t = \nu_{pt}/E_p$. The stress-strain laws reduce to-

$$\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{12}\\ \gamma_{13}\\ \gamma_{23}\end{Bmatrix} = \begin{bmatrix} 1/E_p & -\nu_p/E_p & -\nu_{tp}/E_t & 0 & 0 & 0\\ -\nu_p/E_p & 1/E_p & -\nu_{tp}/E_t & 0 & 0 & 0\\ -\nu_{pt}/E_p & -\nu_{pt}/E_p & 1/E_t & 0 & 0 & 0\\ 0 & 0 & 0 & 1/G_p & 0 & 0\\ 0 & 0 & 0 & 0 & 1/G_t & 0\\ 0 & 0 & 0 & 0 & 0 & 1/G_t \end{bmatrix} \begin{Bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{12}\\ \sigma_{13}\\ \sigma_{23}\end{Bmatrix}$$

Isotropic and anisotropic material properties of Iron are given in TABLE 1 and 2. Isotropic and anisotropic material properties of Cobalt are given in TABLE 3 and 4. Isotropic and anisotropic material properties of Nickel are given in TABLE 5 and 6. These properties are taken from[3].

RESULTS AND DISCUSSION

FE Analyses results in terms of load and stress for the Iron, Cobalt and Nickel considering isotropic and anisotropic conditions at 1 mm displacement are given in TABLE 7 and 8. From the tables it can be observed that load and stress in isotropic case is more than anisotropic case when crystal structure are BCC and FCC and when the crystal structure is HCP the value of load and stress for isotropic and anisotropic cases are comparable. Ratio of anisotropic to isotropic load for the these materials are given in TABLE 7. It can be observed that anisotropy reduces the load in BCC and FCC but it has negligible influenced in HCP structure. It is suggested that load requirement for material deformation should be calculated using actual material parameters. Stresses are also found to be higher in case of isotropic condition. Contour of stresses for Iron, Cobalt and Nickel for isotropic and anisotropic conditions are shown in Figure.3, 4 and 5. From these contours, it can be observed that uniformity of stresses is largely disturbed due to anisotropy for all the three

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materials. In order to make clear idea about the load requirement it is essential to know how load varies with displacement. Load displacement plot for thee three materials considering isotropic and anisotropic cases are shown in Figures 6, 7 and 8. These plots also prove the above statement. Although, Young's moduli are almost equal, load required by isotropic Iron is more than that of isotropic Cobalt due to its low Poisons ratio.

TABLE 1: Isotropic material properties of Iron (BCC)

Density (kg/m^3)	Young's Modulus (GPa)	Poison's Ratio
7850	211	0.29

TABLE 2 : Anisotropic material properties of Iron (BCC)

D_{1111} (GPa)	D_{1212} (GPa)	D_{1122} (GPa)	D_{1313} (GPa)	D_{1133} (GPa)	D_{2222} (GPa)	D_{2323} (GPa)	D_{2233} (GPa)	D_{3333} (GPa)
231.40	116.40	134.70	116.40	134.70	231.40	116.40	134.70	231.40

TABLE 3 : Isotropic material properties of Cobalt (HCP)

Density (kg/m^3)	Young's Modulus (GPa)	Poison's Ratio
8900	209	0.31

TABLE 4 : Anisotropic material properties of Cobalt (HCP)

E_p (E_1,E_2) GPa	E_t(E_3) GPa	υ_p (Nu_{12})	υ_{tp} (Nu_{13})	υ_{pt} (Nu_{23})	G_t(G_{13},G_{23}) GPa	G_p(G_{12}) GPa
211.30	313.15	0.49	0.22	0.15	78.30	71.00

Simulation loads, for isotropic condition, are also compared with theoretical load and are given in TABLE 9. It can be observed that both are almost same which validates the accuracy of simulation. Theoretical stresses are also compared with maximum stresses and given in TABLE 10. It can be observed that maximum stress is localized in a small zone at the outer end of the billet near punch interaction point. In other zones of the billet, stresses developed are almost equal to the theoretical stresses. It is also interesting to observe that under isotropic condition, ratio of maximum stress to theo-

TABLE 5 : Isotropic material properties of Nickel (FCC)

Density (kg/m^3)	Young's Modulus (GPa)	Poison's Ratio
8800	200	0.31

TABLE 6 : Anisotropic material properties of Nickel (FCC)

D_{1111} (GPa)	D_{2222} (GPa)	D_{3333} (GPa)	D_{1212} (GPa)	D_{1313} (GPa)	D_{2323} (GPa)	D_{1122} (GPa)	D_{1133} (GPa)	D_{2233} (GPa)
246.50	246.50	246.50	127.40	127.40	127.40	147.30	147.30	147.30

TABLE 7 : Load at 1 mm displacement

Material	Structure	Load(MN)		Ratio of Load (MN)
		Isotropic Case	Anisotropic Case	Aniso/Iso
Iron	BCC	15.216	9.596	0.630
Cobalt	HCP	15.059	15.845	1.052
Nickel	FCC	14.486	9.959	0.687

TABLE 8 : Stress at 1 mm displacement

Material	Structure	Max. Stress (MPa)		Ratio of Stress (MPa)
		Isotropic Case	Anisotropic Case	Aniso./Iso.
Iron	BCC	1038	611.9	0.589
Cobalt	HCP	1021	1012	0.991
Nickel	FCC	983.1	634.7	0.634

TABLE 9 : Simulation and Theoretical value of load at 1 mm displacement

Material	Simulation value of load (MN)	Theoretical value of load (MN)
Iron	15.216	15.192
Cobalt	15.059	15.048
Nickel	14.486	14.400

TABLE 10 : Simulation and Theoretical value of stress at 1mm displacement

Material	Simulation value of Maximum stress (MPa)	Theoretical value of stress (MPa)	Maximum stress/Theoretical stress
Iron	1038	844	1.23
Cobalt	1021	834	1.23
Nickel	983.1	800	1.23

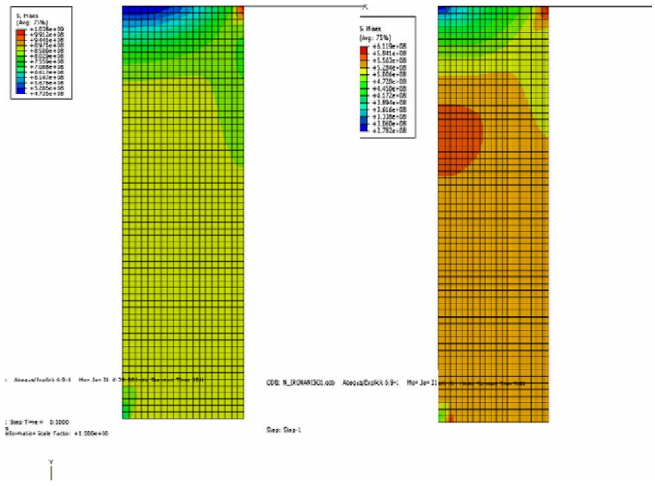

Figure 3 : Contour of stresses for isotropic and anisotropic case of Iron

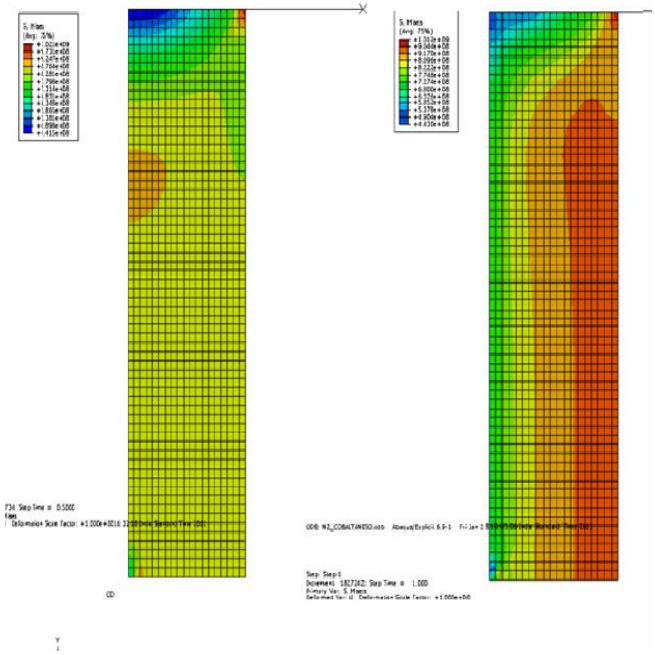

Figure 4 : Contour of stresses for isotropic and anisotropic case of Cobalt

retical stress is constant for all the three material.

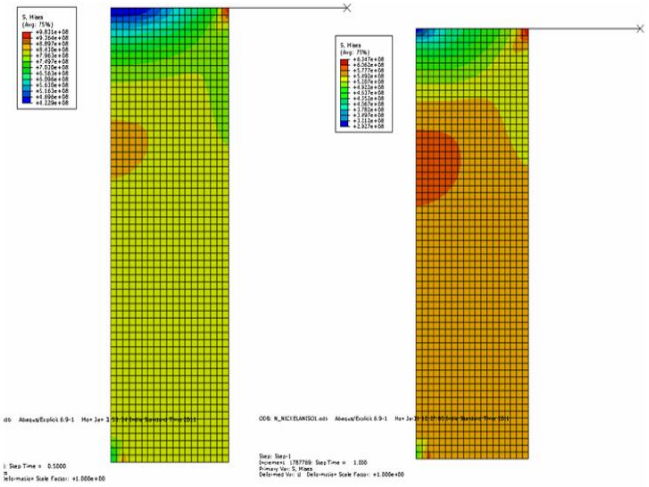

Figure 5 : Contour of stresses for isotropic and anisotropic case of Nickel

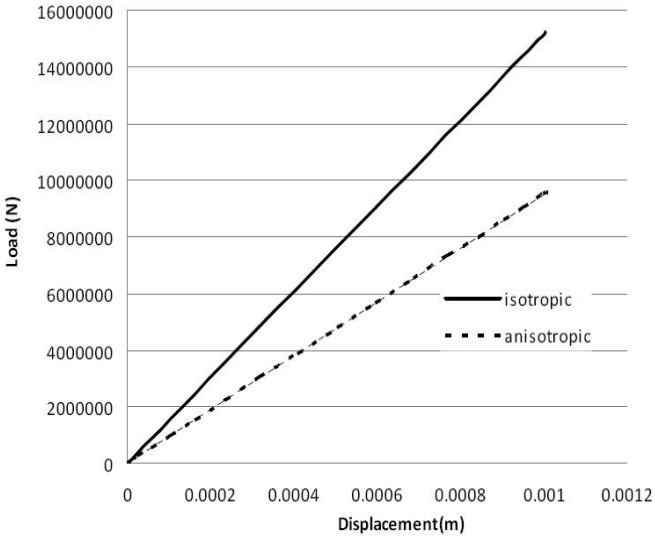

Figure 6 : Load displacement plot for iron (BCC)

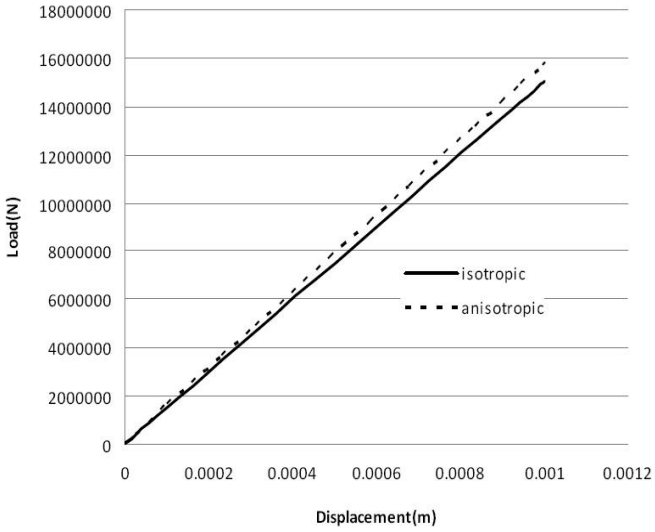

Figure 7 : Load displacement plot for cobalt (HCP)

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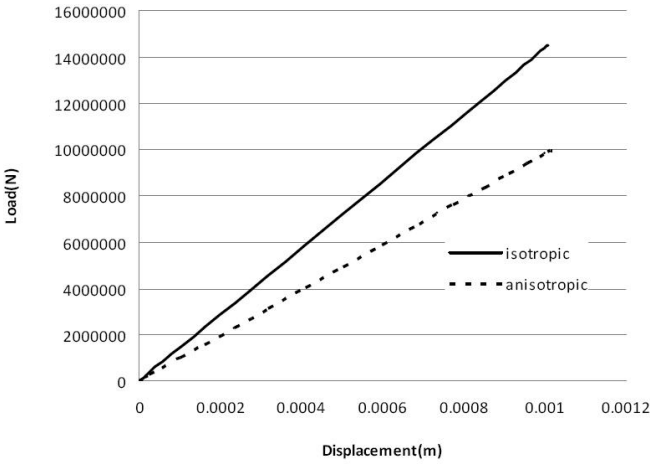

Figure 8 : Load displacement plot for nickel (FCC)

CONCLUSIONS

Following are salient conclusions of this study-

Load in isotropic case is more than anisotropic case when the material structure is BCC or FCC and when the material structure is HCP the value of load for isotropic and anisotropic condition is comparable.

Stress in isotropic case is greater than anisotropic condition when the material structure is BCC or FCC and when the material structure is HCP the value of stress in isotropic and anisotropic condition is comparable.

Ratio of load and stress for anisotropic to isotropic case is maximum for HCP and minimum for BCC.

For constant young's modulus reduction in Poisons ratio reduces the load requirement.

Accurate material parameters should be used for assessing the energy requirement in material deformation.

Load and stresses obtained from simulation are comparable with that of theoretical counterpart.

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