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The anisotropy of deformation behaviors of MgF_2 single crystal

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Abstract
Anisotropy of deformation behaviors limit the high surface quality of Magnesium fluoride (MgF_2) components. Cleavage factor have the relationship with the anisotropy of deformation behaviors of Magnesium fluoride (MgF_2) single crystal, which can influence the manufacturing efficacy and component quality. To determine the reveal anisotropy mechanism of deformation behaviors of the MgF_2 single crystal, the nanoindentation tests were systematically performed on different crystal planes. Besides, the hardness, displacement-load curves, the SEM images of the surface morphologies and cleavage factors under different experimental conditions were obtained. According to compared the experiment results and the cleavage factors under different experimental conditions, the cleavage factor can be used to reflect the activation of the plastic deformation and reveals the anisotropy of deformation behaviors. The theoretical results consisted well with the experimental results, which can improve the manufacturing efficacy and component quality in the manufacturing process of the MgF_2 components.

Anisotropy, Single crystal, Deformation behavior, Cleavage factor

1. Introduction

Magnesium fluoride (MgF_2) single crystal is widely used as infrared optical components because of the extraordinary infrared optical characterization and excellent mechanical strength. However, MgF_2 single crystal is the typical hard-to-machine materials due to the high brittleness, high hardness and anisotropy. Huang et al. carried out the nano scratch tests and found the obvious brittle damage on the surface of the MgF_2 single crystal [1]. Min et al. determined that the ductile-to-brittle depth of MgF_2 single crystal was affected by the crystal orientations [2]. Liu et al. developed an innovative ultrasonic-assisted cutting technology to manufacture the MgF_2 single crystal and obtained the MgF_2 components with high efficacy and high quality. Although numerous researchers have analyzed the mechanical properties and developed the manufacturing technologies, fewer studies focus on revealing the anisotropy of deformation behaviors of the MgF_2. Revealing the anisotropy of deformation behaviors of the MgF_2 can determine the optimal crystal orientation of manufacturing, however, the anisotropy of deformation behaviors mechanism for MgF_2 single crystal is unclear.

The nanoindentation tests can be used to analyze the deformation behaviors. Li et al. conduced the nanoindentation tests and obtained the hardness, elastic modulus, fracture toughness and maximum elastic recovery rate of YAG crystal [4]. According to nanoindentation tests of the Si single crystal, the significant amorphous and nano-crystalline damage in the subsurface region were observed by Yan et al [5]. Zhang et al. conduced the nanoindentation tests to analyze the deformation behaviors of KDP crystal and found that the creep was induced by the dislocation motion [6]. For the single crystal, the cleavage factor is used to estimate the degree of the cleavage fracture. High cleavage factor is more prone to generate the cleavage fracture. Therefore, plenty of studies determined that cleavage factor is related with the anisotropy of the deformation behaviors. Mizumoto et al. carried out the orthogonal cutting experiments of CaF_2 single crystal and determined that the variation of critical cutting depth is consisted with the variation of cleavage factor [7]. Kwon et al. conduced the scratch experiments of sapphire and analyzed the anisotropy of crack initiation by the cleavage factor [8]. Mizumoto et al. discussed the anisotropic ductility of monocrystalline sapphire by the cleavage factor [9]. Although, numerous researches have discussed and analyzed the cleavage factor, fewer studies deeply introduce the cleavage factor into the anisotropy of deformation behaviors.

This study focuses on the revealing the anisotropy mechanism of deformation behaviors of MgF_2 single crystal by cleavage factor. In this work, the nanoindentation tests were carried out on (001) crystal plane, (010) crystal plane and (110) crystal plane to obtain the displacement-load curves and calculate the hardness. Besides, the surface morphologies of nanoindentation tests on (001) crystal plane, (010) crystal plane and (110) crystal plane are measured by the SEM (Scanning Electron Microscope) to analyzed deformation behaviors, and the cleavage factor under different experimental conditions were calculated to analyze and illustrate the anisotropy of the deformation behaviors. This paper reveals the anisotropy mechanism of the deformation behaviors of MgF_2 single crystal, which can provide the theory to suppress the brittle damage and improve the manufacturing efficacy.

2. Experimental methods and simulation models

2.1. Materials and methods

The displacement-load curve can be used to analyze the deformation behaviors. In order to analyze the anisotropy of the deformation behaviors of MgF_2 single crystal, the nanoindentation tests were carried out on the (001) crystal plane, (010) crystal plane and (110) crystal plane to obtain the displacement-load curves. As shown in the Figure. 1, the Berkovich indenter was used to obtain the displacement-load curves under different displacement depth. The dimensions of the workpiece were 10×5×2 mm.

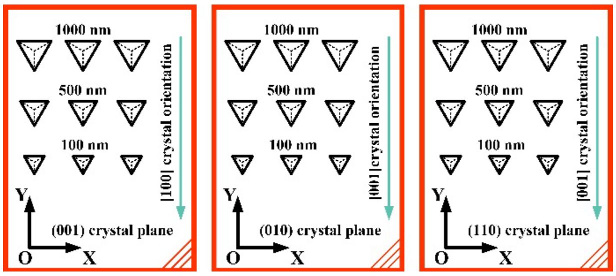

Figure 1. Schematic diagram of the nanoindentation tests on the different crystal planes

The damage of the workpiece surface has a significant effect on the deformation behaviors. Therefore, the chemical-mechanical polishing technology was used to obtain the workpieces with damage-free surface. The quasi-static mode can be used to get the hardness during the nanoindentation tests. The detailed experimental conditions of the nanoindentation tests were listed in Table 1. Each test was repeated three times to confirm the accuracy of the experimental results. Indentation morphologies were observed by the Scanning Electron Microscope (SEM, SUPRA55 SAPPHIRE, Germany).

Table 1 Experimental conditions.

No.	Crystal plane	The maximum Indentation displacement *h*
1-3	(001)	100 nm, 500 nm, 1000 nm
4-6	(010)	100 nm, 500 nm, 1000 nm
7-9	(110)	100 nm, 500 nm, 1000 nm

2.2. The calculation of Hardness and cleavage factors

Hardness is the key mechanical parameter which can reflect the characteristic of the resistance to the deformation. Therefore, the hardness can be used to analyze the anisotropy of the deformation behaviors. The hardness $H=P_m/A_s$, where P_m is the maximum load during the nanoindentation test, and A_s is the contact area between the indenter and workpiece under the P_m. The Berkovich indenter shapes as the triangular pyramid. The angle between the perpendicular line and the edge line is 77.05°and the angle between the perpendicular line and the pyramid plane is 65.3°. According to the geometry of the Berkovich indenter, the $A_s=3\sqrt{3}(h\tan65.3°)/2$。

cleavage factor can be used to represent the degree of the slip motion and cleavage fracture. As shown in the Figure 2, during deformation behaviors of MgF_2 single crystal, the cleavage fracture was induced by the tensile stress σ_k which along the cleavage plane. The higher the cleavage factor is, the more easily the cleavage fracture occur. The cleavage factor $m=\cos^2\alpha$， Where α is the angle between the cleavage plane and the force P.

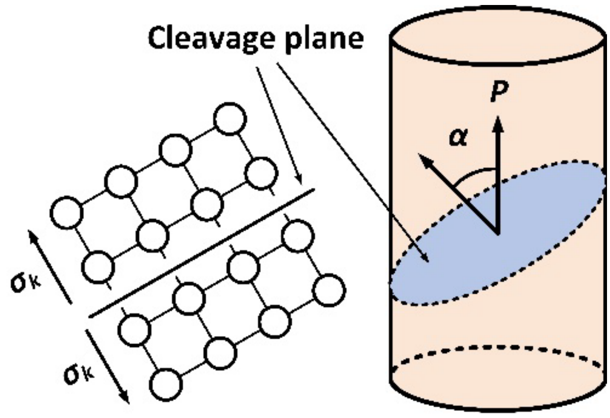

Figure 2. The cleavage fracture

3. Results and disucssions

3.1. Deformation behaviors of MgF_2 single crystal

The hardness curves of (001) crystal plane, (010) crystal plane and (110) crystal plane are shown in Figure 3. Due to the size effect, the hardness *H* increases initially and then decrease with the depth of indentation *h* increasing. When depth of indentation *h* higher than 600 nm, the hardness value turns to be stable. It is clear that the hardness of (001) crystal plane is lowest and the hardness of (110) crystal plane is highest, which indicates that the plastic deformation is most prone to occur on (001) crystal plane and brittle fracture most easily generates on (110) crystal plane.

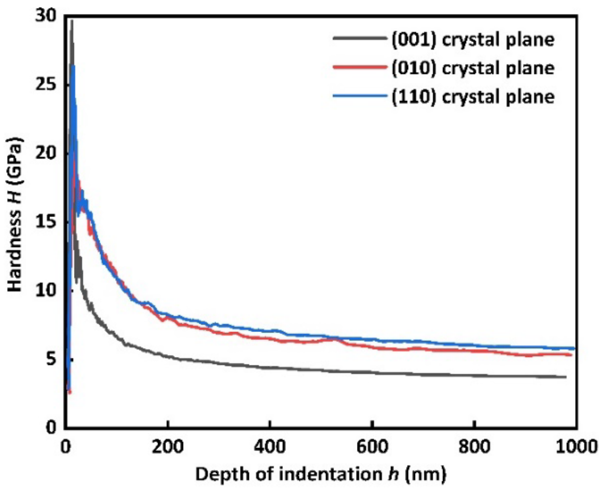

Figure 3. Hardness curves of (001) crystal plane, (010) crystal plane and (110) crystal plane.

The displacement-load curves are shown in the Figure 4. Under the same depth of indentation *h*, the load values of (001) crystal plane, (010) crystal plane and (110) crystal plane are significantly different. the maximum loads of (001) crystal plane, (010) crystal plane and (110) crystal plane are approximately 79.1 mN, 102.1 mN and 112.5 mN, respectively. Compared with the max loads under the same displacement depths, the loads of (001) crystal plane is lowest. Besides, according to the Figure 4 (d)-(f), the "pop-in" which is symbol of the elastic-to-plastic transformation can be observed. However, the depths of "pop-in" occurrence for (001) crystal plane, (010) crystal plane and (110) crystal plane are approximately 14.5 nm, 39.4 nm and 72.8 nm, respectively. Compared with the loads of the "pop-in" occurrence, the loads of (001) crystal plane is lowest. lower the depth of "pop-in" and the loads under the same depth are, the more easily the plastic deformation occur.

The results of the hardness, the load values of the first occurrence of 'pop-in' and max loads of the indentation displacement under the same depth of the displacement can reflect the plastic deformation behaviors. The lower the hardness, the load value of the first occurrence of 'pop-in' and the load under the same indentation displacement are, the more the plastic deformation is prone to generate. Therefore, the plastic deformation is most prone to occur on (001) crystal plane and least prone to occur on (110) crystal plane for MgF_2 single crystal.

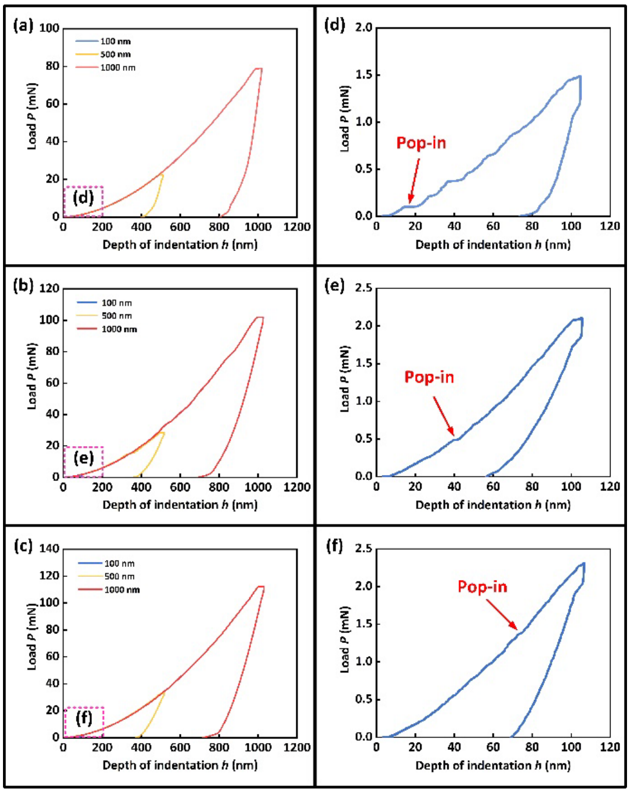

Figure 4. The displacement-load curves of (a) (001) crystal plane, (b) (010) crystal plane and (c) (110) crystal plane. The enlarge displacement-load curves of (d) (001) crystal plane, (e) (010) crystal plane and (f) (110) crystal plane when *h*=100 nm.

3.2. Cleavage factor of different crystal planes

The surface morphologies of (001) crystal plane, (010) crystal plane and (110) crystal plane are shown in the Figure 5. For (001) crystal plane, there are not distinct cracks, which indicates that the plastic derformation play the domain role during the nanoindentation tests. For (010) crystal plane, the cracks are generated when the max depth is 500 nm. With the depths increasing, the cracks propagate. However, the cracks only appear on the one side. For (110) crystal plane, the cracks are generated when the max depth is 500 nm like (010) crystal plane. And the crack appears on the three areas of the surface. Compare with the SEM image of surface morphologies, the cracks of the (110) crystal plane is most severe, and the plastic deformation in most prone to generate on (001) crystal plane.

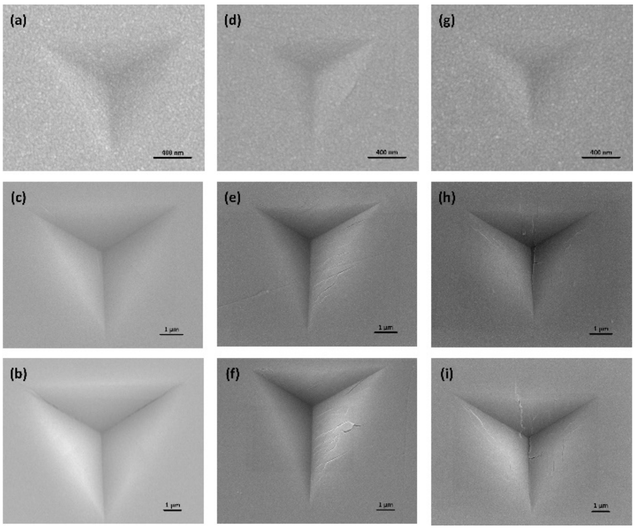

Figure 5. (a), (b) and (c) are the SEM image of surface morphologies on (001) crystal plane under 100 nm, 500 nm and 1000 nm. (d), (e) and (f) are the SEM image of surface morphologies on (010) crystal plane under 100 nm, 500 nm and 1000 nm. (g),(h) and (i) are the SEM image of surface morphologies on (110) crystal plane under 100 nm, 500 nm and 1000 nm.

The higher cleavage factor is, the more cleavage fracture prone to occur. For MgF_2 single crystal, the cleavage plane are (110) crystal plane and $(1\bar{1}0)$ crystal plane [10]. During the nanoindentation tests, only the normal force work on the workpiece. Based on the space and geometric conditions, the cleavage factors under different experimental conditions are calculated and listed in the Table 2. For (001) crystal plane, the cleavage factors of (110) cleavage plane and $(1\bar{1}0)$ cleavage plane are 0, which indicates the cleavage fracture is hard to generate on the (001) crystal plane during the nanoindentation. However, the cleavage factors of (110) cleavage plane and $(1\bar{1}0)$ cleavage plane are 0.5 for (010) crystal plane, which means the degree of the cleavage fracture for (110) cleavage plane and $(1\bar{1}0)$ cleavage plane is same on (010) crystal plane. Besides, for (110) crystal plane, the cleavage factors of (110) cleavage plane is 1, but the cleavage factors of $(1\bar{1}0)$ cleavage plane is 0, which indicates the cleavage fracture of (110) cleavage plane is mainly activated. Compared with the results of the three crystal planes, the cleavage factors for (110) crystal plane are maximum and the cleavage factor for (001) crystal plane is minimum, indicating the (001) crystal plane is most prone to occur the plastic generation, and the cleavage fracture is easiest to generate on (110) crystal plane, which consists with the experimental results. Therefore, the hardness of the (110) crystal plane is highest and the hardness of the (001) crystal plane is lowest. The plastic deformation is most prone to occur on (001) crystal plane, and the cleavage fracture is easiest to generate on (110) crystal plane.

Table 2 The cleavage factor of different crystal plane.

Crystal plane	Cleavage factor of (110) cleavage plane	Cleavage factor of $(1\bar{1}0)$ cleavage plane
(001)	0	0
(010)	0.5	0.5
(110)	1	0

4. Conclusion

In this work, the nanoindentation tests of MgF_2 single crystal were systematically carried out on different crystal planes. The hardness, displacement-load curves, the SEM images of the surface morphologies and cleavage factors under different experimental conditions were obtained to analyze the anisotropy of the deformation behaviors of MgF_2 single crystal. According to the experiment results, the plastic deformation is most prone to occur on (001) crystal plane, and the cleavage fracture is easiest to generate on (110) crystal plane. In addition, the cleavage factors were calculated to analyze the anisotropy of the deformation behaviors. The cleavage factors of (001) crystal plane is 0. However, the maximum cleavage factor is calculated on (110) crystal plane. It is obvious that the activation degree of cleavage fracture is highest for (110) crystal plane and lowest for (001) crystal plane. The cleavage fracture is hard to occur on (001) crystal plane and easy to generate on (110) crystal plane. Therefore, the plastic deformation is easiest to occur on (001) crystal plane.

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