論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Studies on effect of stress and film thickness on domain structure in (100)/(001)-oriented epitaxial tetragonal Pb(Zr,Ti)O 3 films
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出典(和文)	学位:博士(工学), 学位授与機関:東京工業大学, 報告番号:甲第11140号, 授与年月日:2019年3月26日, 学位の種別:課程博士, 審査員:舟窪 浩,松田 晃史,東 正樹,稲邑 朋也,保科 拓也,山田 智明
Citation(English)	Degree:Doctor (Engineering), Conferring organization: Tokyo Institute of Technology, Report number:甲第11140号, Conferred date:2019/3/26, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
Doctoral Program

論 文 要 旨

THESIS SUMMARY

系・コース： Department of, Graduate major in	材料 系 材料 コース	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of （ 工学 ）
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

In this study, we investigated the domain structure of the film grown under tensile strain for $Pb(Zr,Ti)O_3$ films, which is a typical piezoelectric material and ferroelectric material. I mainly investigated the influence of strain and film thickness on the domain structure. The influence of misfit strain was investigated in Chapters 2, 3, and 4, and the influence of the film thickness on the domain structure was investigated in Chapters 5, and 6.

In Chapter 2, the effect of misfit strain to the domain structure was systematically investigated using {100}-oriented epitaxial tetragonal PZT films with various Zr/(Zr+Ti) ratio grown on $(100)KTaO_3$ substrate. In general, studies on the influence of misfit strain have been carried out by adjusting the lattice parameter using different kinds of the substrate. However, systematic investigation is impossible by this method. In Chapter 2, systematic investigation on the influence of misfit strain was carried out by changing the composition of the PZT films grown on $(100)KTaO_3$ substrates. By using this method, it is possible to systematically investigate the domain structure formed under from compressive to tensile strain. The domain structure occurs is composed of *a*/*c*-domain in case of compressive strain, whereas the domain structure is composed of *a*/*a*-domain and *a*/*c*-domain in case of tensile strain. Many theoretical predictions are predicted to be composed of *a*/*c*-domain regardless of tensile and compressive strain. However, this result showed that not only *a*/*c*-domain but also *a*/*a*-domain is formed for the film prepared under tensile strain. The volume fraction of the domain can be controlled continuously by misfit strain and the area mismatch equation. The domain volume fraction under compressive strain follows the above equation, but the domain volume fraction for the films under tensile strain does not follow above equation. Details are given in Chapters 3 and 4.

In Chapter 3, the formation process of domain structure under tensile strain and compressive strain was investigated. The domain structure where compressive strain occurs is changed from paraelectric phase to ferroelectric *c*-domain and then to *a/c*-domain as decreasing temperature. On the other hand, the domain structure where tensile strain occurs is changed from paraelectric phase to ferroelectric *a*/*a*-domain and *a/c* + *a*/*a*-domain as decreasing temperature. The formation process is different under tensile and compressive strain, there is a difference in the domain structure that is ultimately composed due to the difference in formation process. In addition, the influence of the cooling rate was also investigated during the cooling process. The influence of cooling rate was not noticeable in the domain structure under compressive strain, but the effect of cooling rate was observed in

the domain structure under tensile strain. It is influenced kinetically in the domain structure under tensile strain.

In Chapter 4, the domain structure before and after voltage application was investigated for the films prepared under compressive and tensile strain. The domain structure of the film grown under tensile strain composed of *a*/*c*-domain and *a*/*a*-domain, and their lattice parameters are distorted compared to *a*/*c*-domain one for the film formed under compressive strain. The change in the domain volume fraction before and after the application of an electric field under compressive strain was several %, while that of under tensile strain was about 30%. The volume fraction after application of an electric field for the film grown under tensile strain well agrees with the area mismatch equation. By forming *a*/*a*-domain at the first, it is considered that following *a*/*c*-domain formation becomes difficult and it is not sufficiently relaxed. It is considered that it changed to a more stable state by applying an electric field.

In Chapter 5, the film thickness dependence of the domain structure of the film grown under tensile strain was investigated. I investigated mainly thin films below 90 nm in Chapter 5. A thin $PbTiO_3$ film below 90 nm in thickness grown on $KTaO_3$ substrate forms an *a*/*a*-domain. Lattice parameters and tilting angle increase with increasing a film thickness, and these parameters keep constant value in the case of reaching bulk value of *a*-axis one. The tilting angle, *a*, increase with increasing of *c*/*a* ratio following equation: $\alpha = \tan^{-1}(c/a) - 45°$. Domain width of *a*/*a*-domain increase with increasing film thickness, showing the similar behavior followed by Kittel's law, but the thin film thickness is slightly larger due to the influence of *c*/*a* ratio change with film thickness. The phase transition temperature show the the maximum value of 660 °C in case of 30 nm thick film, and the phase transition temperature above 30 nm gradually decreases and approaches to the bulk phase transition temperature due to relaxation of strain. When the film thickness is below 30 nm, it tends to decrease gradually with decreasing film thickness, it may be the effect of general size effect and this is not reported for the films consist of *a*/*a*-domain.

In Chapter 6, the film thickness dependence of the domain structure under tensile strain was investigated. A thick film up to 5300 nm was investigated. In addition, the domain structures of the films grown under tensile and compression strain were compared and comprehensively investigated. The domain structure under compressive strain forms a *c*-domain in the thin film and changes to *a*/*c*-domain, then *a'*/*a'*-domain + *a'*/*c'*-domain as the film thickness increases. On the other hand, the domain structure of the film grown under tensile strain is *a'*/*a'*-domain + *a'*/*c'*-domain + *a''*/*c''*-domain, and then *a'*/*a'*-domain + *a'*/*c'*-domain. The combination of *a'*/*a'*-domain + *a'*/*c'*-domain was formed without a difference in domain structure under compressive and tensile strain in a film thickness of more than 2100 nm.