Effect of addition of elements in group IVB (C, Si, Ge, Sn) on polarity inversion of ScAlN piezoelectric thin films

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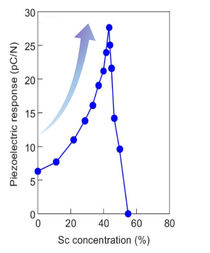
① Why controlling the polarity of ScAlN is important?

Scandium Aluminum Nitride (ScAlN)



(Akiyama et al, *Adv. Mater.*, (2009) 21, 593)

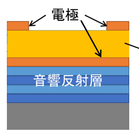
Addition of Sc resulted in 500% enhancement in piezo response d_{33}.

Stacking Al-polar/N-polar resulted in filter that can work at **twice higher** frequency

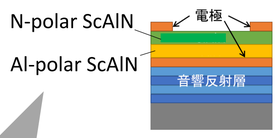
Piezoelectric Stack structure	GeAlN/AlN	AlN/AlN
Total piezo layer thickness (μm)	3.10	3.10
Resonator Frequency (GHz)	2.58	1.39
Resonance mode	2nd over tone	Fundamental

(Mizuno, T. et al. 19th International Conference on Solid-State Sensors, Actuators and Microsystems (TRANSDUCERS), 2017, 1891)


(www.apple.com)



Today's smartphone contains ScAlN-based RF filter



Polarity control technology is needed

Next-generation RF filter

- Twice **Higher** freq.
- **Wider** Bandwidth

Next-generation HEMT

The use of N-polar wide band gap nitride resulted higher conductivity and higher breakdown voltage

(reproduced from 日経エレクトロニクス 2023年2月号)

② Our proposal to control polarity

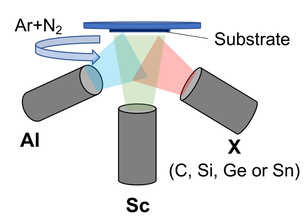
Strategies to control polarity:

- Addition of Silicon (Si)[1] or Germanium (Ge)[2] could inverse the polarity of non-doped AlN to N-polar.

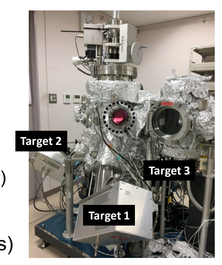
([1]Anggraini et al, Sci. Rep. (2020), [2]Mizuno et al, Transducer (2017))

- Addition of following elements into ScAlN:
  - (1) Carbon (C)
  - (2) Silicon (Si)
  - (3) Germanium (Ge)
  - (4) Tin (Sn)

Thin film deposition



(RF sputtering with multiple targets)



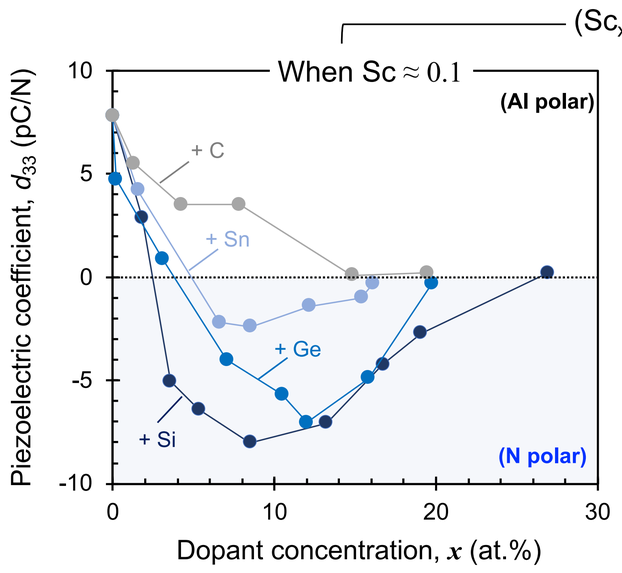
The objective of this work:

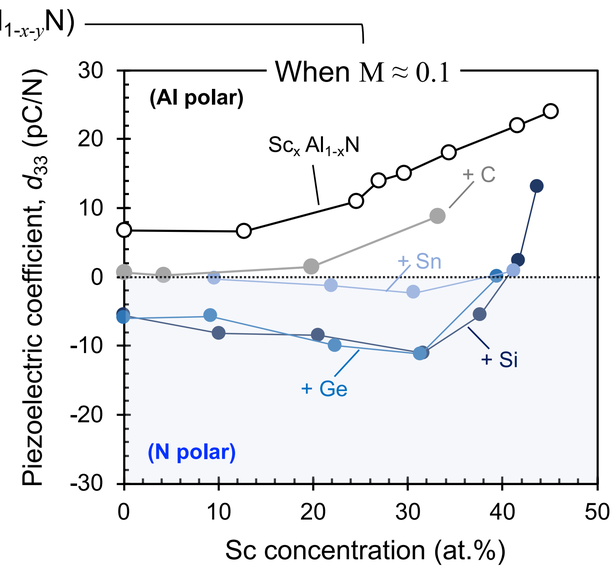
- **Investigate the effect of addition of elements in group IVB on polarity of ScAlN**
- **Elucidate the mechanism for polarity inversion by addition of those elements**

③ Effect of addition of C, Si, Ge, Sn on the polarity of ScAlN thin films

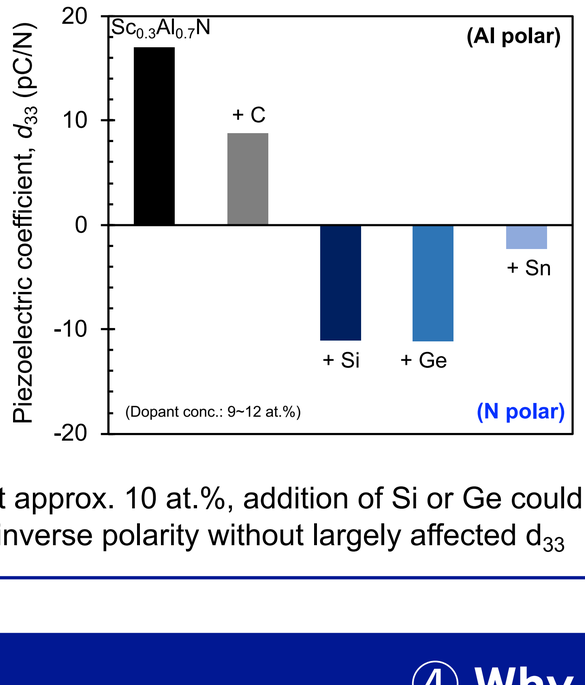
- Not all elements in group IVB could inverse the polarity of ScAlN thin films.

- **Addition of Si, Ge or Sn could inverse the polarity of ScAlN.**
- **Addition of Carbon *could not* inverse the polarity of ScAlN**

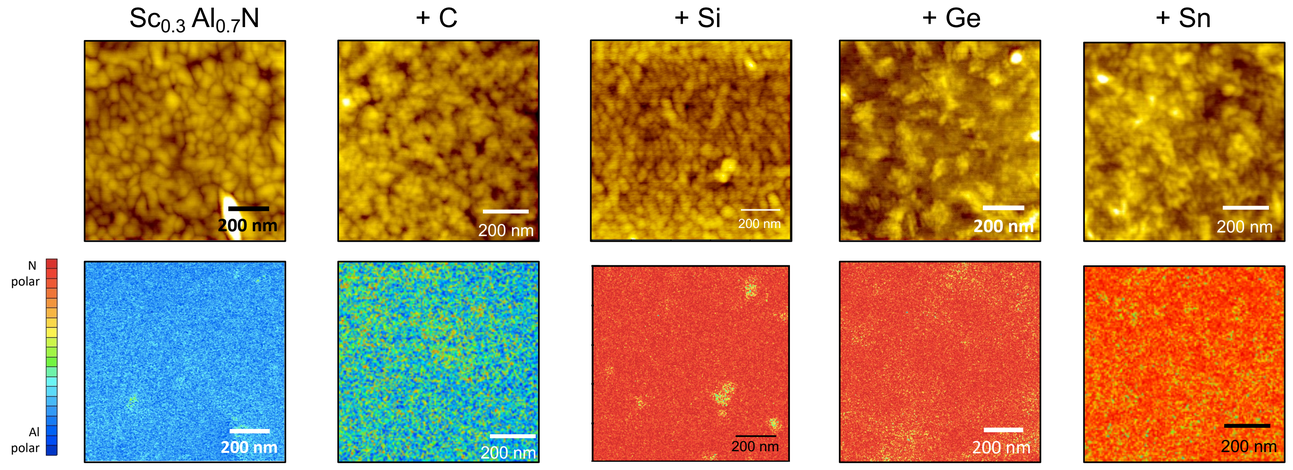




- Addition of Si, Ge or Sn could inverse the polarity of ScAlN thin films **when Sc concentration is lower than 40 at.%.**
- The range of Si, Ge or Sn concentration required to inverse the polarity is not only depending on dopant (M) concentration but also on Sc concentration.



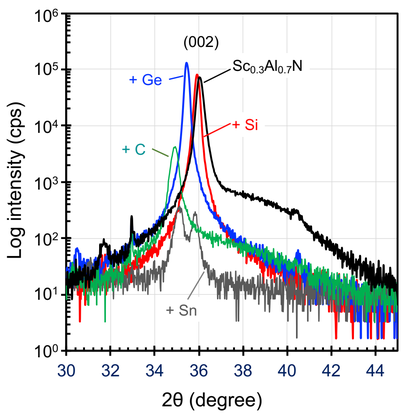
At approx. 10 at.%, addition of Si or Ge could inverse polarity without largely affected d_{33}



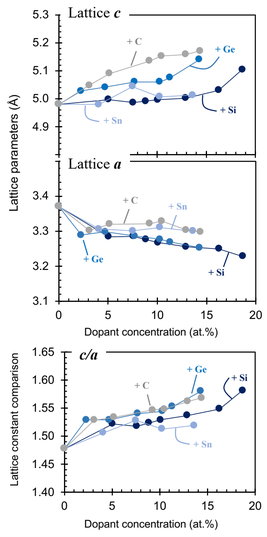
- ➢ Addition of C → mixture which mainly consist of Al-polar and non-polar components.
- ➢ Addition of Si or Ge → mainly consist of N-polar components.
- ➢ Addition of Sn → mixture mainly consist of N-polar as well as fractions of non-polar parts.

Al-polar → **N-polar**

④ Why addition of element can inverse the polarity of ScAlN?

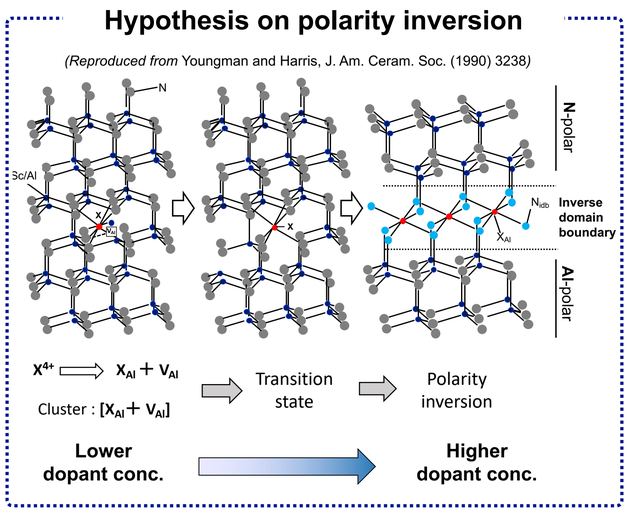


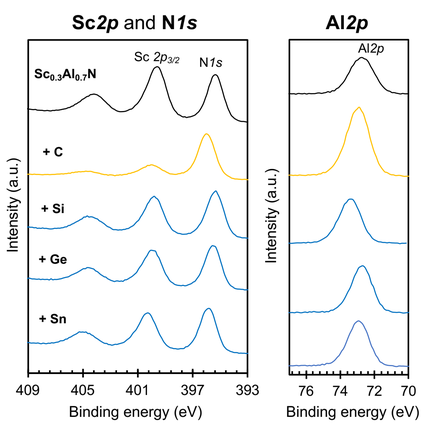
- Addition of of Si or Ge could maintain wurtzite structure with good crystallinity.
- Different elements have different effect on lattice parameters of wurtzite (*c*, *a* and *c/a*).



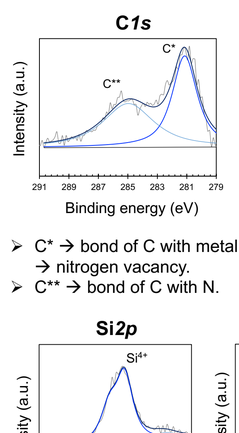
Hypothesis on polarity inversion

(Reproduced from Youngman and Harris, J. Am. Ceram. Soc. (1990) 3238*)*

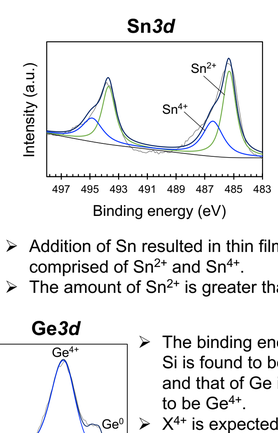




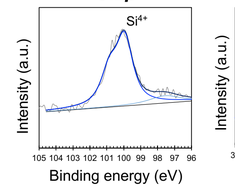
- The binding energy of Al is found to be Al^{3+}.
- The binding energy of Sc is found to be Sc^{3+}.
- Addition of C affect the binding energy of N*1s*.

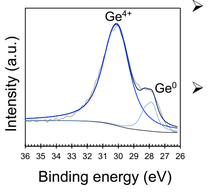


- ➢ C* → bond of C with metal → nitrogen vacancy.
- ➢ C** → bond of C with N.



- ➢ Addition of Sn resulted in thin film comprised of Sn^{2+} and Sn^{4+}.
- ➢ The amount of Sn^{2+} is greater than Sn^{4+}.





- ➢ The binding energy of Si is found to be Si^{4+} and that of Ge is found to be Ge^{4+}.
- ➢ X^{4+} is expected to form cluster with vacancy.

$[X_{Al} + V_{Al}]$

⑤ Conclusions

- The polarity of $Sc_xAl_{1-x}N$ can be controlled by incorporating Si, Ge or Sn but addition of C could not inverse the polarity of thin film.
- The polarity can be managed by controlling the concentration of dopants (Si, Ge, Sn) as well as Sc including their ratios.
- Elements such as Si or Ge are confirmed to exist as X^{4+} which may form a cluster of $[X_{Al}+V_{Al}]$ that could induce polarity inversion.

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産総研
ともに挑む。つぎを創る。