

## Motivation

Dolomite-ankerite solid solutions,  $\text{Ca}(\text{Mg}, \text{Fe})(\text{CO}_3)_2$  (natural samples usually contain minor traces of Mn) constitute up to 50% of the Earth's surface carbonates. Up to now only the elastic tensor of end-member dolomite,  $\text{CaMg}(\text{CO}_3)_2$  was reported. This is the first study on the elastic properties of Fe-dolomite and ankerite. The dependence of the elastic properties on composition is investigated.

## Experimental methods

Natural Fe-dolomite (Ank-1, Ank-2 and Ank4) and ankerite (Ank-5) samples, were characterized by EMPA and PXRD.

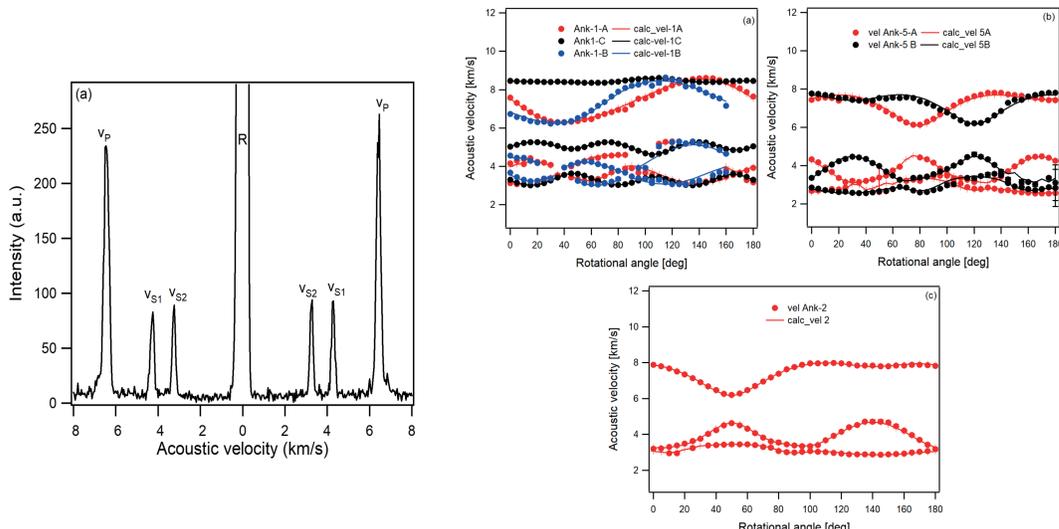
The chemical composition of the samples are:

- **Ank-1**  $\text{Ca}_{0.96}\text{Mg}_{0.99}\text{Fe}_{0.05}(\text{CO}_3)_2$
- **Ank-2**  $\text{Ca}_{0.99}\text{Mg}_{0.55}\text{Fe}_{0.4}\text{Mn}_{0.06}(\text{CO}_3)_2$
- **Ank-4**  $\text{Ca}_{0.89}\text{Mg}_{0.78}\text{Fe}_{0.29}\text{Mn}_{0.03}(\text{CO}_3)_2$
- **Ank-5**  $\text{Ca}_{0.99}\text{Mg}_{0.33}\text{Fe}_{0.63}\text{Mn}_{0.05}(\text{CO}_3)_2$

## Brillouin spectroscopy

The samples Ank-1, Ank-2 and Ank-5 were studied by Brillouin spectroscopy at ambient conditions.

FIG 1: (Left) Brillouin spectrum of Ank1. (Right) Dependence of the acoustic velocities as a function of the rotational angle for different platelets of Ank-1 (a); Ank-5 (b) and Ank-2 (c).



TAB1: Elastic tensor coefficients, bulk modulus (Ks), shear modulus (Gs) and universal anisotropy index (Au) for Fe-dolomite samples Ank-1, Ank-2 and Ank-5 measured in this study, together with literature values [1,2,3,4,5] and values obtained by DFT calculations (this study).

Spez. [1]	Experimental			DFT					
	Ank-1	This work Ank-2	Ank-5	Chen [2]	Humbert [3]	This work	Bakri [4]	Titiloye [5]	
$C_{11}$ (GPa)	206 (1)	204.2(8)	184.1(7)	171(1)	204(2)	205	186(1)	196.6	201.6
$C_{12}$ (GPa)	69(2)	71.7(6)	79(1)	76.0(6)	69(3)	71	62.3(5)	64.6	71.0
$C_{13}$ (GPa)	59(2)	57.0(6)	59(1)	46(4)	57.4	57.4	50.5(5)	54.71	57.4
$C_{14}$ (GPa)	-21(2)	-20.8(4)	-20(78)	-16(9)	20(1)	-19.5	15.28(7)	22.45	-19.5
$C_{15}$ (GPa)	10(3)	10.7(8)	12.4(2)	7(2)	13.7	13.7	-10(3)	-1.35	13.7
$C_{33}$ (GPa)	115 (1)	112.0(3)	95(5)	97(5)	112.8	112.8	102.8(3)	110.01	113.0
$C_{44}$ (GPa)	40.5(4)	40.0(5)	39.4(5)	35.4(3)	39(2)	39.8	37.1(3)	41.57	39.8
$C_{66}$ (GPa)	69(2)	66.2(6)	52(1)	47(1)	62(1)	62(1)	62(1)	62(1)	62(1)
$K_S$ (GPa)	96(6)	94(2)	87(5)	85(9)	95(6)	85(5)	90(6)	94(6)	94(6)
$G_S$ (GPa)	47(7)	46(2)	36(5)	46(8)	47(7)	44(5)	46(7)	46(7)	46(7)
$A^u$	1.34	1.37	1.2			1.01			

## Conclusions

The elastic properties of Fe-dolomite and ankerite are strongly influenced by the different compositions. The substitution of Fe for Mg in the double carbonate produces non-linearities in the bulk modulus that are absent in the  $\text{MgCO}_3$ - $\text{FeCO}_3$  system.

## References

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## Synchrotron powder-XRD

High-pressure PXRD experiments were performed on samples Ank-2, Ank-4 and Ank-5. The samples were loaded in symmetric DAC, using Ne as pressure transmitting medium. A second order Birch-Murnaghan EoS was used to fit the volume data.

## Elastic properties

Non-linear behaviour of the bulk modulus,  $K$ , of dolomite-ankerite solid solutions.

FIG 2: Bulk modulus  $K$  as function of composition for Fe-Ca-Mg carbonate systems

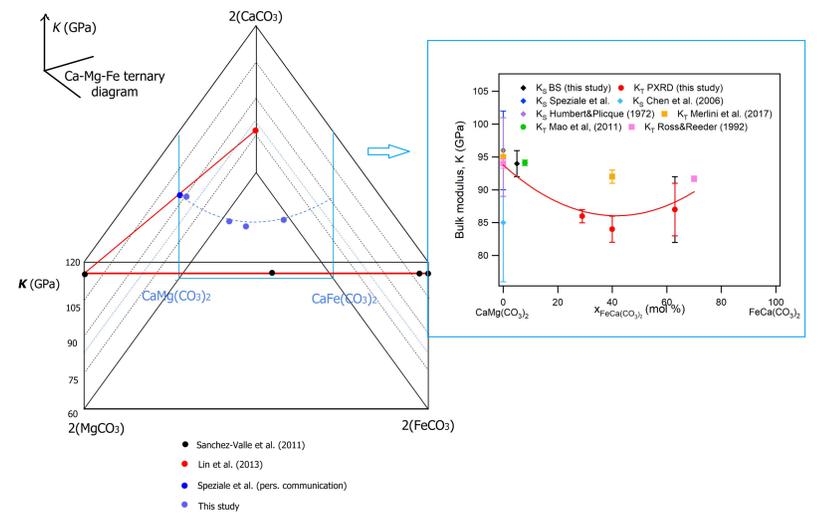


FIG 3: Elastic tensor coefficients of the measured samples Ank-1, Ank-2 and Ank-5, together with the values from Speziale et al. [1] as function of the  $\text{CaFe}(\text{CO}_3)_2$  content,  $x$ .

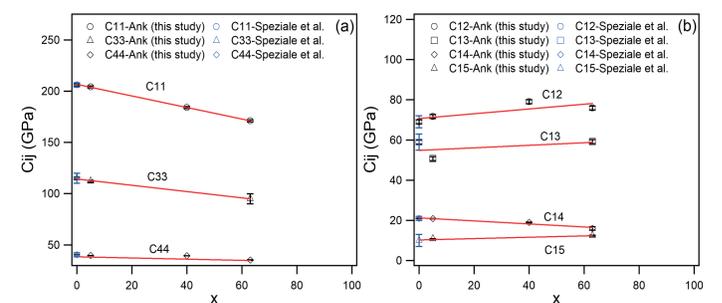
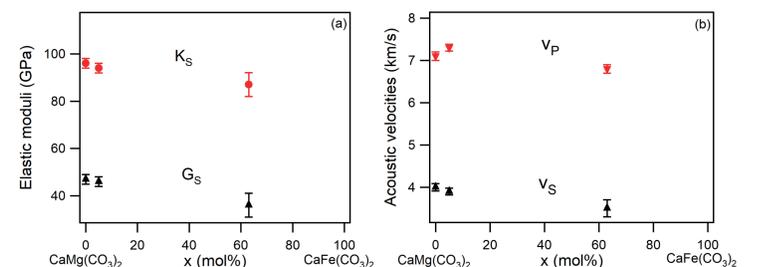


FIG 4: Aggregate properties of Ank-1 and Ank-5 as function of the  $\text{CaFe}(\text{CO}_3)_2$  content, together with the data for  $\text{CaMg}(\text{CO}_3)_2$  from Speziale et al. [1]



## Acknowledgements

We acknowledge funding by DFG (FOR 2125 'CarboPaT', WI1232, SP1216/7-1). DESY is acknowledged for providing the experimental facility. We are thankful to the Museum für Naturkunde of Berlin for providing the samples. We are thankful to Hans-Josef Reichmann, Hanns-Peter Nabein, Franziska Wilke and Eiken Haussühl for their help.