



## Science Arts & Métiers (SAM)

is an open access repository that collects the work of Arts et Métiers Institute of Technology researchers and makes it freely available over the web where possible.

This is an author-deposited version published in: <https://sam.ensam.eu>

Handle ID: <http://hdl.handle.net/10985/24383>



This document is available under CC BY license

### To cite this version :

Charles MAREAU - The dependence of X-ray elastic constants with respect to the penetration depth - Journal of Applied Crystallography - Vol. 56, n°5, p.1446-1455 - 2023



JOURNAL OF  
APPLIED  
CRYSTALLOGRAPHY

**Volume 56 (2023)**

**Supporting information for article:**

**The dependence of X-ray elastic constants with respect to the penetration depth**

**Charles Marea**

Table 1: Surface and bulk X-ray elastic constants for copper ( $A = 0.72$  and  $a = 0.5431$  nm). Single crystal elastic constants were taken from Epstein & Clarkson (1965).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-1.70	-1.93	0.46	7.53	8.23	0.46
{200}	-4.85	-3.76	0.38	16.84	13.71	0.38
{220}	-2.55	-2.39	0.06	9.85	9.60	0.06
{311}	-3.34	-2.90	0.33	12.42	11.13	0.33
{222}	-1.70	-1.93	0.46	7.56	8.23	0.46
{400}	-4.85	-3.76	0.38	16.84	13.71	0.38
{331}	-2.26	-2.26	—	9.20	9.20	—
{420}	-3.31	-2.89	0.33	12.33	11.09	0.33
{422}	-2.55	-2.39	0.06	9.85	9.60	0.06
{333}	-1.70	-1.93	0.46	7.56	8.23	0.46
{511}	-4.16	-3.38	0.37	14.85	12.56	0.37

Table 2: Surface and bulk X-ray elastic constants for aluminium ( $A = 0.02$  and  $a = 0.40498$  nm). Single crystal elastic constants were taken from Thomas (1968).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-4.55	-4.67	0.48	18.03	18.40	0.48
{200}	-5.48	-5.27	0.45	20.83	20.20	0.45
{220}	-4.77	-4.82	0.48	18.86	18.86	—
{311}	-4.99	-4.99	—	19.36	19.36	—
{222}	-4.55	-4.67	0.48	18.03	18.40	0.48
{400}	-5.48	-5.27	0.45	20.83	20.20	0.45
{331}	-4.71	-4.78	0.48	18.51	18.73	0.47
{420}	-4.98	-4.98	—	19.34	19.34	—
{422}	-4.77	-4.82	0.48	18.86	18.86	—
{333}	-4.55	-4.67	0.48	18.03	18.40	0.48
{511}	-5.28	-5.14	0.45	20.22	19.83	0.46

Table 3: Surface and bulk X-ray elastic constants for nickel ( $A = 0.50$  and  $a = 0.35251$  nm). Single crystal elastic constants were taken from Epstein & Clarkson (1965).

$\{hkl\}$	$\bar{s}_{1,hkl} [0]$ TPa $^{-1}$	$\bar{s}_{1,hkl} [\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2} \bar{s}_{2,hkl} [0]$ TPa $^{-1}$	$\frac{1}{2} \bar{s}_{2,hkl} [\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-0.89	-1.02	0.39	4.45	4.84	0.39
{200}	-2.36	-1.91	0.44	8.87	7.52	0.44
{220}	-1.24	-1.24	—	5.51	5.51	—
{311}	-1.65	-1.49	0.53	6.75	6.26	0.53
{222}	-0.89	-1.02	0.39	4.47	4.84	0.39
{400}	-2.36	-1.91	0.44	8.87	7.52	0.44
{331}	-1.13	-1.18	0.17	5.23	5.32	0.16
{420}	-1.63	-1.48	0.53	6.71	6.24	0.53
{422}	-1.24	-1.24	—	5.51	5.51	—
{333}	-0.89	-1.02	0.39	4.47	4.84	0.39
{511}	-2.03	-1.72	0.47	7.91	6.96	0.47

Table 4: Surface and bulk X-ray elastic constants for Fe-18Cr-14Ni alloy ( $A = 0.75$  and  $a = 0.3593$  nm). Single crystal elastic constants were taken from Teklu (2004).

$\{hkl\}$	$\bar{s}_{1,hkl} [0]$ TPa $^{-1}$	$\bar{s}_{1,hkl} [\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2} \bar{s}_{2,hkl} [0]$ TPa $^{-1}$	$\frac{1}{2} \bar{s}_{2,hkl} [\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-0.80	-0.95	0.36	4.64	5.09	0.36
{200}	-2.92	-2.18	0.40	10.98	8.77	0.40
{220}	-1.33	-1.26	0.53	6.23	6.00	0.52
{311}	-1.92	-1.60	0.44	7.98	7.03	0.43
{222}	-0.80	-0.95	0.36	4.65	5.09	0.36
{400}	-2.92	-2.18	0.40	10.98	8.77	0.40
{331}	-1.18	-1.17	1.35	5.74	5.74	—
{420}	-1.90	-1.59	0.44	7.92	7.00	0.44
{422}	-1.33	-1.26	0.53	6.23	6.00	0.52
{333}	-0.80	-0.95	0.36	4.65	5.09	0.36
{511}	-2.41	-1.92	0.51	9.63	7.99	0.51

Table 5: Surface and bulk X-ray elastic constants for  $\alpha$ -iron ( $A = 0.51$  and  $a = 0.28665$  nm). Single crystal elastic constants were taken from Leese & Lord Jr. (1968).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{110}	-1.33	-1.31	0.43	5.92	5.92	—
{200}	-2.54	-2.04	0.37	9.53	8.11	0.37
{211}	-1.33	-1.31	0.43	5.92	5.92	—
{220}	-1.33	-1.31	0.43	5.92	5.92	—
{222}	-0.94	-1.07	0.38	4.83	5.18	0.38
{310}	-2.10	-1.78	0.38	8.26	7.32	0.38
{222}	-0.94	-1.07	0.38	4.83	5.18	0.38
{321}	-1.33	-1.31	0.43	5.92	5.92	—
{400}	-2.54	-2.04	0.37	9.53	8.11	0.37
{330}	-1.33	-1.31	0.43	5.92	5.92	—
{420}	-1.76	-1.58	0.38	7.27	6.71	0.38

Table 6: Surface and bulk X-ray elastic constants for  $\alpha$ -tantalum ( $A = 0.11$  and  $a = 0.33204$  nm). Single crystal elastic constants were taken from Soga (1966)

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{110}	-1.75	-1.75	—	7.00	7.00	—
{200}	-2.32	-2.12	0.43	8.70	8.12	0.43
{211}	-1.75	-1.75	—	7.00	7.00	—
{220}	-1.75	-1.75	—	7.00	7.00	—
{222}	-1.54	-1.62	0.40	6.37	6.62	0.40
{310}	-2.10	-1.99	0.45	8.07	7.71	0.44
{222}	-1.54	-1.62	0.40	6.37	6.62	0.40
{321}	-1.75	-1.75	—	7.00	7.00	—
{400}	-2.32	-2.12	0.43	8.70	8.12	0.43
{330}	-1.75	-1.75	—	7.00	7.00	—
{420}	-1.94	-1.88	0.46	7.58	7.40	0.46

Table 7: Surface and bulk X-ray elastic constants for chromium ( $A = 0.07$  and  $a = 0.28839$  nm). Single crystal elastic constants were taken from Sumer & Smith (1963).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{110}	-0.80	-0.77	0.44	4.59	4.50	0.44
{200}	-0.52	-0.58	0.38	3.76	3.93	0.38
{211}	-0.80	-0.77	0.44	4.59	4.50	0.44
{220}	-0.80	-0.77	0.44	4.59	4.50	0.44
{222}	-0.89	-0.84	0.40	4.87	4.70	0.40
{310}	-0.62	-0.65	0.34	4.06	4.13	0.35
{222}	-0.89	-0.84	0.40	4.87	4.70	0.40
{321}	-0.80	-0.77	0.44	4.59	4.50	0.44
{400}	-0.52	-0.58	0.38	3.76	3.93	0.38
{330}	-0.80	-0.77	0.44	4.59	4.50	0.44
{420}	-0.70	-0.70	—	4.30	4.30	—

Table 8: Surface and bulk X-ray elastic constants for the Ti-27Nb-7Al alloy ( $A = 0.77$  and  $a = 0.3290$  nm). Single crystal elastic constants were taken from Wang *et al.* (2019).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{110}	-5.19	-4.85	0.09	18.18	17.16	0.09
{200}	-9.35	-7.26	0.34	30.26	24.40	0.34
{211}	-5.19	-4.85	0.09	17.74	17.16	0.09
{220}	-5.19	-4.85	0.09	17.74	17.16	0.09
{222}	-3.64	-4.03	0.48	13.52	14.70	0.48
{310}	-7.84	-6.40	0.31	25.73	21.82	0.31
{222}	-3.64	-4.03	0.48	13.52	14.70	0.48
{321}	-5.19	-4.85	0.09	17.74	17.16	0.09
{400}	-9.35	-7.26	0.34	30.26	24.40	0.34
{330}	-5.19	-4.85	0.09	17.74	17.16	0.09
{420}	-6.67	-5.73	0.26	22.24	19.79	0.26

Table 9: Surface and bulk X-ray elastic constants for  $\alpha$ -titanium ( $A = 0.08$ ,  $a = 0.29508$  nm and  $c = 0.46855$  nm). Single crystal elastic constants were taken from Fisher & Renken (1964).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-3.11	-2.96	0.35	12.33	11.98	0.29
{110}	-3.11	-2.96	0.35	12.26	11.98	0.29
{002}	-2.04	-2.33	0.43	9.52	10.14	0.45
{101}	-2.95	-2.89	0.39	11.91	11.76	0.38
{102}	-2.67	-2.72	0.62	11.28	11.28	—
{110}	-3.11	-2.96	0.35	12.26	11.98	0.29
{103}	-2.46	-2.58	0.55	10.63	10.88	0.62
{200}	-3.11	-2.96	0.35	12.26	11.98	0.29
{112}	-2.91	-2.86	0.38	11.81	11.70	0.37
{201}	-3.07	-2.95	0.37	12.17	11.93	0.32
{004}	-2.04	-2.33	0.43	9.52	10.14	0.45
{202}	-2.95	-2.89	0.39	11.91	11.76	0.38
{104}	-2.33	-2.50	0.51	10.28	10.63	0.56
{203}	-2.80	-2.80	—	11.53	11.53	—
{120}	-3.11	-2.96	0.35	12.26	11.98	0.29
{211}	-3.09	-2.95	0.36	12.21	11.95	0.32
{114}	-2.59	-2.67	0.58	11.00	11.13	0.66
{105}	-2.24	-2.45	0.49	10.06	10.49	0.53
{122}	-3.01	-2.92	0.39	12.05	11.86	0.35

Table 10: Surface and bulk X-ray elastic constants for magnesium ( $A = 0.02$ ,  $a = 0.32094$  nm and  $c = 0.52108$  nm). Single crystal elastic constants were taken from Wazzan & Robinson (1967).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-6.49	-6.49	—	28.76	28.76	—
{110}	-6.49	-6.49	—	28.76	28.76	—
{002}	-5.36	-5.77	0.43	25.82	26.88	0.44
{101}	-6.83	-6.73	0.35	29.54	29.54	—
{102}	-6.69	-6.69	—	29.49	29.49	—
{110}	-6.49	-6.49	—	28.76	28.76	—
{103}	-6.37	-6.45	0.54	28.81	28.81	—
{200}	-6.49	-6.49	—	28.76	28.76	—
{112}	-6.87	-6.75	0.36	29.94	29.62	0.36
{201}	-6.58	-6.58	—	29.06	29.06	—
{004}	-5.36	-5.77	0.43	25.82	26.88	0.44
{202}	-6.83	-6.73	0.35	29.54	29.54	—
{104}	-6.07	-6.25	0.47	27.84	28.25	0.52
{203}	-6.87	-6.76	0.36	30.00	29.68	0.36
{120}	-6.49	-6.49	—	28.76	28.76	—
{211}	-6.55	-6.55	—	28.95	28.95	—
{114}	-6.62	-6.62	—	29.29	29.29	—
{105}	-5.87	-6.12	0.45	27.28	27.87	0.48
{122}	-6.74	-6.67	0.33	29.33	29.33	—

Table 11: Surface and bulk X-ray elastic constants for silicon ( $A = 0.11$  and  $a = 0.5431$  nm). Single crystal elastic constants were taken from McSkimin & Andreatch Jr (1964)

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-1.05	-1.14	0.49	6.54	6.83	0.49
{220}	-1.25	-1.28	1.21	7.17	7.25	1.22
{311}	-0.43	-1.43	-0.01	7.88	7.71	-0.01
{400}	-1.93	-1.70	0.31	9.14	8.49	0.31
{331}	-1.19	-1.24	0.76	6.99	7.13	0.77
{422}	-1.25	-1.28	1.21	7.17	7.25	1.22
{333}	-1.05	-1.14	0.49	6.55	6.83	0.49
{511}	-1.74	-1.58	0.24	8.56	8.14	0.24
{440}	-1.25	-1.28	1.21	7.17	7.25	1.22
{531}	-1.34	-1.34	—	7.44	7.44	—
{620}	-1.69	-1.55	0.21	8.40	8.04	0.21

Table 12: Surface and bulk X-ray elastic constants for  $\alpha$ -zinc ( $A = 0.64$ ,  $a = 0.26649$  nm and  $c = 0.49468$  nm). Single crystal elastic constants were taken from Alers & Neighbours (1908).

$\{hkl\}$	$\bar{s}_{1,hkl} [0]$ TPa $^{-1}$	$\bar{s}_{1,hkl} [\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2} \bar{s}_{2,hkl} [0]$ TPa $^{-1}$	$\frac{1}{2} \bar{s}_{2,hkl} [\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-2.47	-2.42	0.73	10.90	10.90	—
{110}	-2.47	-2.42	0.73	10.90	10.90	—
{002}	-5.51	-3.90	0.34	23.14	18.50	0.37
{101}	-2.07	-2.28	0.10	10.68	11.05	0.16
{102}	-2.42	-2.42	—	12.35	12.35	—
{110}	-2.47	-2.42	0.73	10.90	10.90	—
{103}	-3.10	-2.77	0.42	15.15	14.01	0.44
{200}	-2.47	-2.42	0.73	10.90	10.90	—
{112}	-2.05	-2.28	0.11	10.76	11.17	0.15
{201}	-2.36	-2.36	—	10.83	10.89	0.05
{004}	-5.51	-3.90	0.34	23.14	18.50	0.37
{202}	-2.07	-2.28	0.10	10.68	11.05	0.16
{104}	-3.75	-3.07	0.37	17.40	15.29	0.40
{203}	-2.01	-2.30	0.07	11.20	11.57	0.03
{120}	-2.47	-2.42	0.73	10.90	10.90	—
{211}	-2.38	-2.38	—	10.89	10.89	—
{114}	-2.60	-2.52	0.89	13.22	12.88	0.69
{105}	-4.21	-3.29	0.35	18.95	16.16	0.38
{122}	-2.22	-2.31	0.13	10.69	10.93	0.15

Table 13: Surface and bulk X-ray elastic constants for  $\alpha$ -zirconium ( $A = 0.05$ ,  $a = 0.3232$  nm and  $c = 0.5147$  nm). Single crystal elastic constants were taken from Fisher & Renken (1964).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-3.22	-3.34	0.07	13.94	13.60	-0.04
{110}	-3.22	-3.34	0.07	13.48	13.60	-0.04
{002}	-2.65	-2.88	0.44	11.28	11.96	0.43
{101}	-3.67	-3.60	0.64	14.56	14.33	0.65
{102}	-3.71	-3.61	0.65	14.55	14.27	0.64
{110}	-3.22	-3.34	0.07	13.48	13.60	-0.04
{103}	-3.42	-3.42	—	13.66	13.66	—
{200}	-3.22	-3.34	0.07	13.48	13.60	-0.04
{112}	-3.72	-3.63	0.59	14.68	14.41	0.58
{201}	-3.44	-3.44	—	13.89	13.89	—
{004}	-2.65	-2.88	0.44	11.28	11.96	0.43
{202}	-3.67	-3.60	0.64	14.56	14.33	0.65
{104}	-3.27	-3.27	—	13.01	13.16	0.05
{203}	-3.76	-3.66	0.57	14.77	14.45	0.56
{120}	-3.22	-3.34	0.07	13.48	13.60	-0.04
{211}	-3.40	-3.40	—	13.78	13.78	—
{114}	-3.63	-3.55	0.76	14.31	14.09	0.76
{105}	-3.04	-3.16	0.20	12.53	12.83	0.24
{122}	-3.53	-3.53	—	14.14	14.14	—

Table 14: Surface and bulk X-ray elastic constants for germanium ( $A = 0.14$  and  $a = 0.5658$  nm). Single crystal elastic constants were taken from Bogardus (1965).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-1.16	-1.27	0.41	7.92	8.25	0.41
{220}	-1.46	-1.46	—	8.81	8.81	—
{311}	-1.78	-1.67	0.44	9.78	9.45	0.45
{400}	-2.34	-2.04	0.44	11.45	10.56	0.43
{331}	-1.37	-1.40	0.36	8.54	8.65	0.36
{422}	-1.46	-1.46	—	8.81	8.81	—
{333}	-1.16	-1.27	0.41	7.92	8.25	0.41
{511}	-2.09	-1.87	0.44	10.70	10.06	0.44
{440}	-1.46	-1.46	—	8.81	8.81	—
{531}	-1.59	-1.54	0.48	9.21	9.08	0.47
{620}	-2.02	-1.82	0.44	10.49	9.92	0.44

Table 15: Surface and bulk X-ray elastic constants for cadmium telluride ( $A = 0.38$  and  $a = 0.648$  nm). Single crystal elastic constants were taken from Deligoz *et al.* (2006).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-6.48	-7.22	0.43	27.35	29.56	0.43
{200}	-14.06	-11.76	0.37	49.83	43.18	0.37
{220}	-8.24	-8.35	0.84	32.74	32.96	0.84
{311}	-10.27	-9.61	0.35	38.84	36.75	0.35
{222}	-6.48	-7.22	0.43	27.47	29.56	0.43
{400}	-14.06	-11.76	0.37	49.83	43.18	0.37
{420}	-10.21	-9.57	0.35	38.64	36.62	0.35
{422}	-8.24	-8.35	0.84	32.74	32.96	0.84
{440}	-8.24	-8.35	0.84	32.74	32.96	0.84
{600}	-14.06	-11.76	0.37	49.83	43.18	0.37
{442}	-7.25	-7.72	0.47	29.79	31.07	0.47

Table 16: Surface and bulk X-ray elastic constants for titanium carbide ( $A = 0.01$  and  $a = 0.43186$  nm). Single crystal elastic constants were taken from Gilman & Roberts (1961).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-0.48	-0.47	0.48	2.80	2.80	—
{200}	-0.42	-0.43	0.49	2.62	2.66	0.49
{220}	-0.46	-0.46	—	2.77	2.77	—
{311}	-0.45	-0.45	—	2.73	2.73	—
{222}	-0.48	-0.47	0.48	2.80	2.80	—
{400}	-0.42	-0.43	0.49	2.62	2.66	0.49
{331}	-0.47	-0.47	—	2.78	2.78	—
{420}	-0.45	-0.45	—	2.73	2.73	—
{422}	-0.46	-0.46	—	2.77	2.77	—
{333}	-0.48	-0.47	0.48	2.80	2.80	—
{511}	-0.43	-0.44	0.47	2.69	2.69	—

Table 17: Surface and bulk X-ray elastic constants for 2H silicon carbide ( $A = 0.08$ ,  $a = 0.30763$  nm and  $c = 0.50486$  nm). Single crystal elastic constants were taken from Pizzagalli (2021).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-0.27	-0.29	0.44	2.32	2.40	0.48
{002}	-0.20	-0.24	0.40	2.10	2.22	0.39
{101}	-0.39	-0.38	0.35	2.69	2.64	0.33
{102}	-0.44	-0.40	0.33	2.82	2.72	0.35
{2-10}	-0.27	-0.29	0.44	2.32	2.40	0.48
{103}	-0.39	-0.37	0.21	2.66	2.61	0.27
{2-12}	-0.41	-0.39	0.36	2.75	2.68	0.35
{201}	-0.31	-0.32	0.49	2.46	2.49	0.59
{203}	-0.44	-0.40	0.36	2.82	2.73	0.36
{210}	-0.27	-0.29	0.44	2.32	2.40	0.48
{211}	-0.29	-0.31	0.47	2.41	2.45	0.53
{114}	-0.43	-0.39	0.30	2.78	2.70	0.34
{105}	-0.30	-0.30	0.92	2.39	2.43	0.62
{212}	-0.35	-0.35	—	2.58	2.57	0.04
{300}	-0.27	-0.29	0.44	2.32	2.40	0.48
{213}	-0.41	-0.39	0.36	2.74	2.68	0.35
{214}	-0.44	-0.40	0.36	2.82	2.73	0.36

Table 18: Surface and bulk X-ray elastic constants for 4H silicon carbide ( $A = 0.06$ ,  $a = 0.30784$  nm and  $c = 1.00776$  nm). Single crystal elastic constants were taken from Pizzagalli (2021).

$\{hkl\}$	$\bar{s}_{1,hkl} [0]$ TPa $^{-1}$	$\bar{s}_{1,hkl} [\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2} \bar{s}_{2,hkl} [0]$ TPa $^{-1}$	$\frac{1}{2} \bar{s}_{2,hkl} [\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{102}	-0.38	-0.37	0.42	2.67	2.62	0.41
{103}	-0.42	-0.39	0.38	2.77	2.69	0.39
{104}	-0.42	-0.39	0.33	2.77	2.68	0.34
{105}	-0.41	-0.37	0.27	2.71	2.63	0.27
{110}	-0.28	-0.30	0.41	2.37	2.41	0.42
{106}	-0.39	-0.35	0.20	2.63	2.57	0.19
{202}	-0.32	-0.32	0.40	2.49	2.49	—
{205}	-0.41	-0.38	0.40	2.73	2.66	0.40
{206}	-0.42	-0.39	0.38	2.77	2.69	0.39
{109}	-0.30	-0.31	-0.10	2.43	2.43	—
{212}	-0.30	-0.31	0.41	2.46	2.46	—
{213}	-0.33	-0.33	—	2.51	2.51	—
{1010}	-0.30	-0.30	—	2.40	2.40	—
{214}	-0.35	-0.35	0.43	2.58	2.56	0.39
{215}	-0.38	-0.36	0.42	2.65	2.61	0.40
{300}	-0.28	-0.30	0.41	2.37	2.41	0.42
{209}	-0.42	-0.38	0.30	2.74	2.65	0.31

Table 19: Surface and bulk X-ray elastic constants for 6H silicon carbide ( $A = 0.05$ ,  $a = 0.30793$  nm and  $c = 1.51091$  nm). Single crystal elastic constants were taken from Pizzagalli (2021).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{101}	-0.30	-0.31	0.24	2.42	2.46	0.29
{006}	-0.20	-0.24	0.40	2.11	2.22	0.37
{102}	-0.34	-0.34	—	2.54	2.54	—
{103}	-0.38	-0.36	0.58	2.66	2.62	0.53
{104}	-0.40	-0.38	0.46	2.73	2.66	0.45
{107}	-0.39	-0.37	0.36	2.69	2.63	0.44
{108}	-0.38	-0.36	0.34	2.64	2.60	0.45
{2-10}	-0.28	-0.30	0.30	2.38	2.43	0.35
{109}	-0.36	-0.35	0.30	2.59	2.56	0.49
{2-16}	-0.39	-0.37	0.50	2.70	2.64	0.49
{208}	-0.40	-0.38	0.46	2.73	2.66	0.45
{209}	-0.41	-0.38	0.43	2.74	2.67	0.44
{211}	-0.28	-0.30	0.29	2.38	2.43	0.34
{213}	-0.30	-0.31	0.21	2.44	2.47	0.28
{1015}	-0.29	-0.30	0.50	2.36	2.40	0.33
{217}	-0.36	-0.36	0.73	2.62	2.59	0.60
{219}	-0.39	-0.37	0.51	2.69	2.64	0.49

Table 20: Surface and bulk X-ray elastic constants for 3C silicon carbide ( $A = 0.18$  and  $a = 0.4348$  nm). Single crystal elastic constants were taken from Pizzagalli (2021).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-0.18	-0.22	0.34	2.10	2.22	0.34
{200}	-0.56	-0.47	0.36	3.24	2.96	0.36
{220}	-0.27	-0.28	0.11	2.38	2.41	0.11
{311}	-0.38	-0.35	0.47	2.70	2.61	0.47
{222}	-0.18	-0.22	0.34	2.11	2.22	0.34
{400}	-0.56	-0.47	0.36	3.24	2.96	0.36
{331}	-0.24	-0.26	0.24	2.30	2.35	0.24
{420}	-0.37	-0.35	0.48	2.69	2.61	0.47
{422}	-0.27	-0.28	0.11	2.38	2.41	0.11
{333}	-0.18	-0.22	0.34	2.11	2.22	0.34
{511}	-0.48	-0.42	0.39	3.00	2.81	0.39

Table 21: Surface and bulk X-ray elastic constants for tungsten carbide ( $A = 0.07$ ,  $a = 0.29059$  nm and  $c = 0.28367$  nm). Single crystal elastic constants were taken from Lee & Gilmore (1982).

$\{hkl\}$	$\bar{s}_{1,hkl} [0]$ TPa $^{-1}$	$\bar{s}_{1,hkl} [\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2} \bar{s}_{2,hkl} [0]$ TPa $^{-1}$	$\frac{1}{2} \bar{s}_{2,hkl} [\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{001}	-0.32	-0.33	0.35	1.60	1.64	0.38
{100}	-0.38	-0.36	0.46	1.96	1.91	0.44
{101}	-0.31	-0.32	0.19	1.68	1.70	0.21
{110}	-0.38	-0.36	0.46	1.96	1.91	0.44
{002}	-0.32	-0.33	0.35	1.61	1.64	0.38
{111}	-0.34	-0.34	—	1.79	1.79	—
{200}	-0.38	-0.36	0.46	1.96	1.91	0.44
{102}	-0.31	-0.32	0.38	1.60	1.64	0.39
{201}	-0.35	-0.34	1.17	1.82	1.82	—
{112}	-0.31	-0.32	0.28	1.65	1.68	0.30
{210}	-0.38	-0.36	0.46	1.96	1.91	0.44
{003}	-0.32	-0.33	0.35	1.61	1.64	0.38
{202}	-0.31	-0.32	0.19	1.68	1.70	0.21
{211}	-0.36	-0.35	0.72	1.88	1.85	0.63
{103}	-0.31	-0.32	0.38	1.60	1.64	0.38
{300}	-0.38	-0.36	0.46	1.96	1.91	0.44
{301}	-0.36	-0.35	0.64	1.89	1.86	0.58

Table 22: Surface and bulk X-ray elastic constants for silicon nitride ( $A = 0.14$ ,  $a = 0.76044$  nm and  $c = 0.29075$  nm). Single crystal elastic constants were taken from Vogelgesang *et al.* (2000).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{100}	-0.82	-0.82	—	3.80	3.80	—
{110}	-0.82	-0.82	—	3.80	3.80	—
{200}	-0.82	-0.82	—	3.80	3.80	—
{101}	-0.73	-0.75	1.58	3.40	3.48	1.23
{210}	-0.82	-0.82	—	3.80	3.80	—
{301}	-1.01	-0.96	0.36	4.32	4.16	0.38
{221}	-1.01	-0.95	0.40	4.30	4.15	0.40
{320}	-0.82	-0.82	—	3.80	3.80	—
{002}	-0.48	-0.58	0.56	2.64	2.93	0.54
{231}	-0.98	-0.93	0.45	4.22	4.10	0.41
{411}	-0.97	-0.93	0.46	4.20	4.09	0.42
{330}	-0.82	-0.82	—	3.80	3.80	—
{212}	-0.83	-0.83	—	3.71	3.71	—
{511}	-0.94	-0.91	0.49	4.11	4.03	0.41
{430}	-0.82	-0.82	—	3.80	3.80	—
{232}	-0.99	-0.94	0.21	4.22	4.08	0.30
{142}	-1.00	-0.95	0.24	4.25	4.10	0.32
{610}	-0.82	-0.82	—	3.80	3.80	—
{521}	-0.92	-0.89	0.51	4.06	4.00	0.40

Table 23: Surface and bulk X-ray elastic constants for titanium nitride ( $A = 0.06$  and  $a = 0.424$  nm). Single crystal elastic constants were taken from Fodil *et al.* (2014).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-0.64	-0.60	0.43	2.95	2.85	0.43
{200}	-0.41	-0.45	0.40	2.29	2.40	0.40
{220}	-0.58	-0.56	0.57	2.78	2.74	0.58
{311}	-0.51	-0.52	0.14	2.59	2.61	0.15
{222}	-0.64	-0.60	0.43	2.95	2.85	0.43
{400}	-0.41	-0.45	0.40	2.29	2.40	0.40
{331}	-0.59	-0.58	0.50	2.83	2.77	0.51
{420}	-0.51	-0.52	0.13	2.60	2.62	0.13
{422}	-0.58	-0.56	0.57	2.78	2.74	0.58
{333}	-0.64	-0.60	0.43	2.95	2.85	0.43
{511}	-0.46	-0.48	0.34	2.42	2.50	0.34

Table 24: Surface and bulk X-ray elastic constants for  $\alpha$ -corundum ( $A = 0.07$ ,  $a = 0.47606$  nm and  $c = 1.2994$  nm). Single crystal elastic constants were taken from Tefft (1966).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{012}	-0.51	-0.54	0.13	2.85	2.93	0.13
{104}	-0.67	-0.64	0.62	3.37	3.26	0.62
{110}	-0.55	-0.55	—	2.95	2.95	—
{113}	-0.62	-0.61	0.96	3.19	3.13	0.97
{024}	-0.51	-0.54	0.13	2.88	2.93	0.13
{116}	-0.62	-0.61	1.01	3.22	3.16	0.95
{214}	-0.67	-0.64	0.65	3.33	3.22	0.65
{300}	-0.55	-0.55	—	2.95	2.95	—
{226}	-0.62	-0.61	0.96	3.19	3.13	0.97
{2110}	-0.65	-0.62	0.72	3.31	3.22	0.70
{1310}	-0.57	-0.57	—	3.04	3.04	—
{3012}	-0.67	-0.64	0.62	3.37	3.26	0.62
{2014}	-0.53	-0.55	0.16	2.99	3.02	0.06
{416}	-0.69	-0.65	0.60	3.38	3.25	0.60
{4010}	-0.74	-0.68	0.45	3.57	3.38	0.45
{330}	-0.55	-0.55	—	2.95	2.95	—

Table 25: Surface and bulk X-ray elastic constants for cubic zirconia ( $A = 0.52$  and  $a = 0.509$  nm). Single crystal elastic constants were taken from Kandil *et al.* (1984).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{111}	-2.10	-1.79	0.39	8.00	7.06	0.39
{200}	-0.71	-0.87	0.50	3.82	4.28	0.50
{220}	-1.77	-1.56	0.30	6.90	6.35	0.30
{311}	-1.47	-1.30	0.06	5.76	5.57	0.05
{222}	-2.10	-1.79	0.39	7.94	7.06	0.39
{400}	-0.71	-0.87	0.50	3.82	4.28	0.50
{331}	-1.86	-1.62	0.33	7.20	6.56	0.33
{420}	-1.46	-1.30	0.07	5.80	5.60	0.07
{422}	-1.77	-1.56	0.30	6.90	6.35	0.30
{333}	-2.10	-1.79	0.39	7.94	7.06	0.39
{511}	-1.00	-1.06	0.94	4.69	4.85	0.93
{440}	-1.77	-1.56	0.30	6.90	6.35	0.30
{531}	-1.61	-1.45	0.24	6.43	6.03	0.24
{442}	-1.95	-1.69	0.35	7.48	6.75	0.35
{600}	-0.71	-0.87	0.50	3.82	4.28	0.50
{620}	-1.09	-1.11	2.11	4.94	5.02	2.14
{533}	-1.92	-1.66	0.34	7.36	6.67	0.34

Table 26: Surface and bulk X-ray elastic constants for tetragonal zirconia ( $A = 0.23$ ,  $a = 0.3579$  nm and  $c = 0.5165$  nm). Single crystal elastic constants were taken from Kisi & Howard (1998).

$\{hkl\}$	$\bar{s}_{1,hkl}[0]$ TPa $^{-1}$	$\bar{s}_{1,hkl}[\infty]$ TPa $^{-1}$	$k_{1,hkl}$	$\frac{1}{2}\bar{s}_{2,hkl}[0]$ TPa $^{-1}$	$\frac{1}{2}\bar{s}_{2,hkl}[\infty]$ TPa $^{-1}$	$k_{2,hkl}$
{101}	-1.53	-1.45	0.29	6.81	6.55	0.31
{002}	-0.74	-0.93	0.41	4.91	5.39	0.39
{110}	-1.57	-1.47	0.23	6.67	6.44	0.21
{112}	-1.77	-1.61	0.39	7.62	7.14	0.39
{200}	-0.92	-1.02	0.61	4.75	5.11	0.59
{103}	-1.26	-1.26	—	6.28	6.28	—
{211}	-1.49	-1.42	0.23	6.53	6.33	0.21
{202}	-1.53	-1.45	0.29	6.81	6.55	0.31
{004}	-0.74	-0.93	0.41	4.91	5.39	0.39
{220}	-1.57	-1.47	0.23	6.67	6.44	0.21
{213}	-1.71	-1.58	0.41	7.45	7.02	0.41
{301}	-1.06	-1.12	0.86	5.21	5.42	0.77
{204}	-1.51	-1.43	0.24	6.93	6.69	0.28
{312}	-1.47	-1.40	0.21	6.51	6.33	0.20
{105}	-0.99	-1.09	0.55	5.58	5.81	0.58
{224}	-1.77	-1.61	0.39	7.62	7.14	0.39
{400}	-0.92	-1.02	0.61	4.75	5.11	0.59
{215}	-1.49	-1.41	0.19	6.89	6.66	0.25
{314}	-1.66	-1.54	0.41	7.29	6.91	0.41