Table 1. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $GaN_xAs_{1-x}/GaAs$ for different strain states s computed within LDA using 5000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.03842E-3 | 1.02588E-3 | 1.06949E-3 | 1.04769E-3 |
| | $p_2$ | -3.86248E-2 | -4.59965E-2 | -6.35115E-2 | -2.20804E-2 |
| | $p_3$ | -8.80587E-1 | -1.06997E+0 | -1.34430E+0 | -6.46214E-1 |
| | $p_4$ | 3.86596E+0 | 3.86592E+0 | 3.86690E+0 | 3.86670E+0 |
| | $\sigma$ | 1.18159E-3 | 8.42658E-4 | 1.19382E-3 | 9.15397E-4 |
| As | $p_1$ | 1.06816E-3 | 1.04699E-3 | 2.85095E-4 | 1.07483E-3 |
| | $p_2$ | -8.16608E-2 | -1.20145E-1 | -2.73290E-1 | -4.15695E-2 |
| | $p_3$ | -9.55385E-1 | -1.13767E+0 | -1.33618E+0 | -7.20527E-1 |
| | $p_4$ | 4.25073E+0 | 4.25299E+0 | 4.24644E+0 | 4.24734E+0 |
| | $\sigma$ | 2.51771E-3 | 2.52869E-3 | 1.06964E-3 | 1.59468E-3 |
| GaN | | | | | |
| Ga | $p_1$ | 1.05424E-3 | 1.05662E-3 | 1.06819E-3 | 1.03949E-3 |
| | $p_2$ | -5.27738E-2 | -6.37576E-2 | -8.11920E-2 | -3.67438E-2 |
| | $p_3$ | -9.20624E-1 | -1.13022E+0 | -1.43385E+0 | -6.61840E-1 |
| | $p_4$ | 3.97876E+0 | 3.98074E+0 | 3.98263E+0 | 3.97760E+0 |
| | $\sigma$ | 1.63237E-3 | 1.55445E-3 | 2.00603E-3 | 8.87785E-4 |
| N | $p_1$ | 6.59401E-4 | 1.03776E-3 | 1.23707E-3 | 1.09651E-3 |
| | $p_2$ | -8.02212E-2 | -7.95578E-2 | -1.02854E-1 | -2.72472E-2 |
| | $p_3$ | -2.10070E-1 | -2.58821E-1 | -3.30213E-1 | -2.13758E-1 |
| | $p_4$ | 1.38685E+0 | 1.39224E+0 | 1.40229E+0 | 1.39074E+0 |
| | $\sigma$ | 1.52871E-3 | 6.62364E-3 | 1.92194E-2 | 4.57462E-3 |

Table 2. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $GaN_xAs_{1-x}/GaAs$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.02387E-3 | 1.02145E-3 | 1.06838E-3 | 1.04954E-3 |
| | $p_2$ | -3.97432E-2 | -4.62031E-2 | -6.37383E-2 | -2.19771E-2 |
| | $p_3$ | -8.79266E-1 | -1.06933E+0 | -1.34409E+0 | -6.46107E-1 |
| | $p_4$ | 3.86566E+0 | 3.86595E+0 | 3.86681E+0 | 3.86678E+0 |
| | $\sigma$ | 1.21225E-3 | 8.03359E-4 | 1.13108E-3 | 8.85770E-4 |
| As | $p_1$ | 1.06667E-3 | 1.04714E-3 | 2.80100E-4 | 1.06759E-3 |
| | $p_2$ | -8.17187E-2 | -1.20157E-1 | -2.73993E-1 | -4.20518E-2 |
| | $p_3$ | -9.55324E-1 | -1.13787E+0 | -1.33561E+0 | -7.20695E-1 |
| | $p_4$ | 4.25112E+0 | 4.25320E+0 | 4.24637E+0 | 4.24752E+0 |
| | $\sigma$ | 2.63054E-3 | 2.59490E-3 | 1.03679E-3 | 1.44128E-3 |
| GaN | | | | | |
| Ga | $p_1$ | 1.05436E-3 | 1.08137E-3 | 1.07218E-3 | 1.03949E-3 |
| | $p_2$ | -5.27922E-2 | -6.23101E-2 | -8.08219E-2 | -3.67336E-2 |
| | $p_3$ | -9.19949E-1 | -1.13080E+0 | -1.43472E+0 | -6.61850E-1 |
| | $p_4$ | 3.97848E+0 | 3.98049E+0 | 3.98315E+0 | 3.97761E+0 |
| | $\sigma$ | 1.56255E-3 | 1.49296E-3 | 2.13355E-3 | 8.91004E-4 |
| N | $p_1$ | 6.71383E-4 | 1.03290E-3 | 1.20109E-3 | 1.09070E-3 |
| | $p_2$ | -8.00925E-2 | -8.05290E-2 | -2.07182E-1 | -2.74286E-2 |
| | $p_3$ | -2.10003E-1 | -2.56694E-1 | -2.24140E-1 | -2.13923E-1 |
| | $p_4$ | 1.38678E+0 | 1.39174E+0 | 1.38458E+0 | 1.39071E+0 |
| | $\sigma$ | 1.57573E-3 | 7.21451E-3 | 2.44570E-3 | 4.24737E-3 |

Table 3. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $GaN_xAs_{1-x}/GaAs$ for different strain states s computed within GGA using 5000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.07197E-3 | 1.03681E-3 | 1.05925E-3 | 1.06610E-3 |
| | $p_2$ | -3.46482E-2 | -4.14069E-2 | -5.99361E-2 | -2.02353E-2 |
| | $p_3$ | -8.89160E-1 | -1.08021E+0 | -1.35510E+0 | -6.51472E-1 |
| | $p_4$ | 3.86859E+0 | 3.86873E+0 | 3.86951E+0 | 3.86929E+0 |
| | $\sigma$ | 1.25109E-3 | 8.46729E-4 | 8.52038E-4 | 8.79693E-4 |
| As | $p_1$ | 1.07064E-3 | 1.05556E-3 | 6.81591E-4 | 1.07216E-3 |
| | $p_2$ | -8.24256E-2 | -1.17619E-1 | -2.79523E-1 | -4.23672E-2 |
| | $p_3$ | -9.57021E-1 | -1.14442E+0 | -1.33381E+0 | -7.21035E-1 |
| | $p_4$ | 4.25340E+0 | 4.25677E+0 | 4.24855E+0 | 4.24926E+0 |
| | $\sigma$ | 2.65003E-3 | 2.89150E-3 | 1.05823E-3 | 1.52844E-3 |
| GaN | | | | | |
| Ga | $p_1$ | 1.05385E-3 | 1.01705E-3 | 1.06391E-3 | 1.05065E-3 |
| | $p_2$ | -5.20069E-2 | -6.96674E-2 | -8.03517E-2 | -3.58416E-2 |
| | $p_3$ | -9.24960E-1 | -1.12818E+0 | -1.44004E+0 | -6.66043E-1 |
| | $p_4$ | 3.98023E+0 | 3.98086E+0 | 3.98408E+0 | 3.97966E+0 |
| | $\sigma$ | 1.53382E-3 | 1.15768E-3 | 1.88878E-3 | 9.66786E-4 |
| N | $p_1$ | 7.79309E-4 | 7.85448E-4 | 1.25996E-3 | 1.03039E-3 |
| | $p_2$ | -8.00901E-2 | -1.19576E-1 | -2.11641E-1 | -2.66946E-2 |
| | $p_3$ | -1.99793E-1 | -2.06320E-1 | -2.04915E-1 | -2.06919E-1 |
| | $p_4$ | 1.37165E+0 | 1.37087E+0 | 1.36925E+0 | 1.37578E+0 |
| | $\sigma$ | 1.64504E-3 | 1.28470E-3 | 2.56099E-3 | 4.53519E-3 |

Table 4. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $GaN_xAs_{1-x}/GaAs$ for different strain states s computed within GGA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.07270E-3 | 1.03933E-3 | 1.05669E-3 | 1.06610E-3 |
| | $p_2$ | -3.47364E-2 | -4.14547E-2 | -6.00611E-2 | -2.02353E-2 |
| | $p_3$ | -8.89151E-1 | -1.08062E+0 | -1.35485E+0 | -6.51472E-1 |
| | $p_4$ | 3.86867E+0 | 3.86903E+0 | 3.86928E+0 | 3.86929E+0 |
| | $\sigma$ | 1.23812E-3 | 8.05943E-4 | 9.13306E-4 | 8.79693E-4 |
| As | $p_1$ | 1.07600E-3 | 1.05556E-3 | 7.25804E-4 | 1.07216E-3 |
| | $p_2$ | -8.17826E-2 | -1.17588E-1 | -2.79525E-1 | -4.23672E-2 |
| | $p_3$ | -9.57359E-1 | -1.14441E+0 | -1.33390E+0 | -7.21035E-1 |
| | $p_4$ | 4.25310E+0 | 4.25667E+0 | 4.24850E+0 | 4.24926E+0 |
| | $\sigma$ | 2.60315E-3 | 2.91055E-3 | 1.06801E-3 | 1.52844E-3 |
| GaN | | | | | |
| Ga | $p_1$ | 1.05374E-3 | 1.01693E-3 | 1.06370E-3 | 1.05065E-3 |
| | $p_2$ | -5.19830E-2 | -6.96003E-2 | -8.03855E-2 | -3.58416E-2 |
| | $p_3$ | -9.25032E-1 | -1.12838E+0 | -1.44011E+0 | -6.66043E-1 |
| | $p_4$ | 3.98023E+0 | 3.98115E+0 | 3.98413E+0 | 3.97966E+0 |
| | $\sigma$ | 1.53247E-3 | 1.23048E-3 | 1.92012E-3 | 9.66786E-4 |
| N | $p_1$ | 1.04277E-3 | 8.45330E-4 | 1.25238E-3 | 1.03039E-3 |
| | $p_2$ | -8.08957E-2 | -1.20145E-1 | -9.01140E-2 | -2.66946E-2 |
| | $p_3$ | -1.99292E-1 | -2.05926E-1 | -3.28838E-1 | -2.06919E-1 |
| | $p_4$ | 1.37169E+0 | 1.37086E+0 | 1.39104E+0 | 1.37578E+0 |
| | $\sigma$ | 1.61020E-3 | 1.33710E-3 | 2.29570E-2 | 4.53519E-3 |

Table 5. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $Al_xGa_{1-x}As/GaAs$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| AlAs | | | | | |
| Al | $p_1$ | 1.03115E-3 | 1.00000E-3 | 1.00000E-3 | 1.00000E-3 |
| | $p_2$ | -2.51212E-3 | 1.45843E-4 | 2.76150E-4 | 1.42077E-4 |
| | $p_3$ | 6.06196E-3 | 8.11407E-3 | 9.83967E-3 | 5.51188E-3 |
| | $p_4$ | 2.47332E+0 | 2.47236E+0 | 2.47235E+0 | 2.47235E+0 |
| | $\sigma$ | 8.88564E-4 | 4.62001E-4 | 5.14123E-4 | 4.60912E-4 |
| As | $p_1$ | 1.03115E-3 | 1.00000E-3 | 1.01255E-3 | 1.00000E-3 |
| | $p_2$ | -4.00925E-3 | 2.30239E-4 | 4.54282E-4 | 2.47154E-4 |
| | $p_3$ | 5.33996E-3 | 7.84340E-3 | 9.26861E-3 | 5.58281E-3 |
| | $p_4$ | 4.21451E+0 | 4.21277E+0 | 4.21204E+0 | 4.21286E+0 |
| | $\sigma$ | 8.90454E-4 | 2.91723E-4 | 1.95312E-4 | 2.95643E-4 |
| GaAs | | | | | |
| Ga | $p_1$ | 1.03115E-3 | 1.01255E-3 | 1.01255E-3 | 1.00000E-3 |
| | $p_2$ | -3.81498E-3 | 2.44400E-4 | 2.79156E-4 | 1.52194E-4 |
| | $p_3$ | 5.52353E-3 | 8.17886E-3 | 9.88736E-3 | 5.35467E-3 |
| | $p_4$ | 3.86636E+0 | 3.86410E+0 | 3.86410E+0 | 3.86485E+0 |
| | $\sigma$ | 8.84772E-4 | 2.02173E-4 | 1.96960E-4 | 2.97709E-4 |
| As | $p_1$ | 1.03115E-3 | 1.00000E-3 | 1.01255E-3 | 1.00000E-3 |
| | $p_2$ | -4.19662E-3 | 2.43588E-4 | 3.83956E-4 | 2.34673E-4 |
| | $p_3$ | 5.60379E-3 | 8.16784E-3 | 9.78622E-3 | 5.76360E-3 |
| | $p_4$ | 4.24452E+0 | 4.24286E+0 | 4.24203E+0 | 4.24286E+0 |
| | $\sigma$ | 8.84768E-4 | 2.92538E-4 | 1.95313E-4 | 2.90605E-4 |

Table 6. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $GaSb_xAs_{1-x}/GaAs$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.10198E-3 | 1.03344E-3 | 1.06721E-3 | 1.04539E-3 |
| | $p_2$ | 3.51901E-3 | 5.43412E-3 | 1.10049E-2 | 7.98224E-3 |
| | $p_3$ | 3.26709E-1 | 3.96961E-1 | 4.96726E-1 | 2.33674E-1 |
| | $p_4$ | 3.86777E+0 | 3.86752E+0 | 3.86781E+0 | 3.86836E+0 |
| | $\sigma$ | 1.23633E-3 | 1.06077E-3 | 1.29469E-3 | 1.10888E-3 |
| As | $p_1$ | 9.24129E-4 | 1.00538E-3 | 1.03702E-3 | 1.06363E-3 |
| | $p_2$ | 6.97981E-5 | -7.53967E-4 | 2.20791E-3 | 6.31967E-3 |
| | $p_3$ | 3.34887E-1 | 3.95950E-1 | 4.79455E-1 | 2.55310E-1 |
| | $p_4$ | 4.24677E+0 | 4.24672E+0 | 4.24773E+0 | 4.24640E+0 |
| | $\sigma$ | 1.28893E-3 | 1.04733E-3 | 1.26669E-3 | 9.92092E-4 |
| GaSb | | | | | |
| Ga | $p_1$ | 1.07371E-3 | 1.01580E-3 | 1.03509E-3 | 1.05074E-3 |
| | $p_2$ | 6.00727E-3 | 8.91380E-3 | 1.52275E-2 | 9.71073E-3 |
| | $p_3$ | 3.16895E-1 | 3.82021E-1 | 4.73586E-1 | 2.30538E-1 |
| | $p_4$ | 3.79959E+0 | 3.79904E+0 | 3.79985E+0 | 3.79981E+0 |
| | $\sigma$ | 1.36528E-3 | 1.26510E-3 | 1.50718E-3 | 1.18427E-3 |
| Sb | $p_1$ | 1.00180E-3 | 1.03685E-3 | 9.70703E-4 | 1.03965E-3 |
| | $p_2$ | -5.17490E-4 | -3.47218E-3 | 2.40778E-3 | 8.14632E-3 |
| | $p_3$ | 4.86591E-1 | 5.82955E-1 | 7.10874E-1 | 3.63427E-1 |
| | $p_4$ | 6.37368E+0 | 6.37363E+0 | 6.37578E+0 | 6.37331E+0 |
| | $\sigma$ | 1.15941E-3 | 8.82182E-4 | 1.06990E-3 | 8.04220E-4 |

Table 7. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $In_xGa_{1-x}P/GaP$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaP | | | | | |
| Ga | $p_1$ | 1.02067E-3 | 1.03148E-3 | 1.03886E-3 | 1.02777E-3 |
| | $p_2$ | -4.34322E-3 | 1.88488E-2 | 3.61238E-2 | -2.30292E-3 |
| | $p_3$ | 3.38662E-1 | 3.96801E-1 | 5.08890E-1 | 2.40180E-1 |
| | $p_4$ | 3.76819E+0 | 3.76919E+0 | 3.76566E+0 | 3.77021E+0 |
| | $\sigma$ | 1.44844E-3 | 9.26630E-4 | 1.70274E-3 | 9.29603E-4 |
| P | $p_1$ | 1.01672E-3 | 1.02678E-3 | 1.03100E-3 | 1.02120E-3 |
| | $p_2$ | -8.65240E-3 | 9.24674E-3 | 1.71283E-2 | -4.15041E-3 |
| | $p_3$ | 2.98653E-1 | 3.38127E-1 | 4.21253E-1 | 2.25762E-1 |
| | $p_4$ | 2.81360E+0 | 2.81544E+0 | 2.81254E+0 | 2.81576E+0 |
| | $\sigma$ | 1.62262E-3 | 1.16116E-3 | 1.79597E-3 | 1.25671E-3 |
| InP | | | | | |
| In | $p_1$ | 1.02739E-3 | 1.03929E-3 | 1.00998E-3 | 1.02994E-3 |
| | $p_2$ | -7.54157E-3 | 2.18498E-2 | 4.20749E-2 | -2.84988E-3 |
| | $p_3$ | 4.59085E-1 | 5.40256E-1 | 6.92875E-1 | 3.24873E-1 |
| | $p_4$ | 5.83179E+0 | 5.83283E+0 | 5.82899E+0 | 5.83409E+0 |
| | $\sigma$ | 1.31866E-3 | 7.04336E-4 | 1.28480E-3 | 7.04391E-4 |
| P | $p_1$ | 1.01161E-3 | 1.01515E-3 | 1.03367E-3 | 1.02232E-3 |
| | $p_2$ | -1.05967E-2 | 8.41584E-3 | 1.42497E-2 | -4.90408E-3 |
| | $p_3$ | 2.96321E-1 | 3.31184E-1 | 4.10140E-1 | 2.26656E-1 |
| | $p_4$ | 2.75510E+0 | 2.75665E+0 | 2.75400E+0 | 2.75715E+0 |
| | $\sigma$ | 1.77288E-3 | 1.38131E-3 | 2.16814E-3 | 1.46476E-3 |

Table 8. *Table of polynomial coefficients for the modified atomic scattering amplitudes of strained $GaAs_xSb_{1-x}/GaSb$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaAs | | | | | |
| Ga | $p_1$ | 1.05021E-3 | 1.08763E-3 | 1.07076E-3 | 1.09423E-3 |
| | $p_2$ | -7.18356E-3 | -5.20289E-3 | -3.48251E-3 | -3.42260E-3 |
| | $p_3$ | -3.23995E-1 | -3.92564E-1 | -4.88293E-1 | -2.40524E-1 |
| | $p_4$ | 4.10837E+0 | 4.10820E+0 | 4.10759E+0 | 4.10889E+0 |
| | $\sigma$ | 1.19276E-3 | 6.50007E-4 | 7.44514E-4 | 8.28958E-4 |
| As | $p_1$ | 1.06030E-3 | 1.05521E-3 | 1.06958E-3 | 1.06305E-3 |
| | $p_2$ | -1.17725E-2 | -1.22057E-2 | -1.62624E-2 | -5.62987E-3 |
| | $p_3$ | -3.31759E-1 | -3.91378E-1 | -4.76701E-1 | -2.57267E-1 |
| | $p_4$ | 4.50684E+0 | 4.50657E+0 | 4.50705E+0 | 4.50663E+0 |
| | $\sigma$ | 1.18164E-3 | 6.59441E-4 | 6.07604E-4 | 7.69297E-4 |
| GaSb | | | | | |
| Ga | $p_1$ | 1.07833E-3 | 1.05763E-3 | 9.76146E-4 | 1.06769E-3 |
| | $p_2$ | -5.74876E-3 | -2.55939E-3 | 3.32815E-5 | -1.96384E-3 |
| | $p_3$ | -3.17157E-1 | -3.81054E-1 | -4.70815E-1 | -2.39782E-1 |
| | $p_4$ | 4.03856E+0 | 4.03808E+0 | 4.03778E+0 | 4.03910E+0 |
| | $\sigma$ | 1.44463E-3 | 7.58618E-4 | 8.23866E-4 | 9.27152E-4 |
| Sb | $p_1$ | 1.04650E-3 | 1.04591E-3 | 1.06154E-3 | 1.05648E-3 |
| | $p_2$ | -1.63079E-2 | -1.91182E-2 | -2.39255E-2 | -8.41635E-3 |
| | $p_3$ | -4.80884E-1 | -5.72191E-1 | -7.04076E-1 | -3.65150E-1 |
| | $p_4$ | 6.74365E+0 | 6.74357E+0 | 6.74382E+0 | 6.74323E+0 |
| | $\sigma$ | 1.05479E-3 | 5.52395E-4 | 5.21204E-4 | 5.78969E-4 |

Table 9. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $Ga_xIn_{1-x}P/InP$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| GaP | | | | | |
| Ga | $p_1$ | 1.04163E-3 | 1.00546E-3 | 1.01403E-3 | 1.04870E-3 |
| | $p_2$ | -2.68821E-3 | 6.93109E-3 | 1.52592E-2 | -1.40045E-2 |
| | $p_3$ | -3.18674E-1 | -3.91867E-1 | -4.87335E-1 | -2.25894E-1 |
| | $p_4$ | 4.00582E+0 | 4.00539E+0 | 4.00149E+0 | 4.00738E+0 |
| | $\sigma$ | 1.23888E-3 | 1.19083E-3 | 2.09663E-3 | 8.20472E-4 |
| P | $p_1$ | 1.02697E-3 | 1.06015E-3 | 1.02737E-3 | 1.06029E-3 |
| | $p_2$ | -6.83580E-3 | -1.78932E-4 | 3.81800E-3 | -1.50091E-2 |
| | $p_3$ | -2.78728E-1 | -3.32783E-1 | -4.04192E-1 | -2.08474E-1 |
| | $p_4$ | 3.03631E+0 | 3.03612E+0 | 3.03363E+0 | 3.03651E+0 |
| | $\sigma$ | 1.33165E-3 | 1.05971E-3 | 1.85270E-3 | 9.79578E-4 |
| InP | | | | | |
| In | $p_1$ | 1.02498E-3 | 1.00590E-3 | 1.01590E-3 | 1.05481E-3 |
| | $p_2$ | -6.12717E-3 | 6.03015E-3 | 1.42633E-2 | -1.81458E-2 |
| | $p_3$ | -4.36617E-1 | -5.34391E-1 | -6.66614E-1 | -3.05860E-1 |
| | $p_4$ | 6.15587E+0 | 6.15329E+0 | 6.14852E+0 | 6.15478E+0 |
| | $\sigma$ | 1.22557E-3 | 8.47201E-4 | 1.57671E-3 | 6.36553E-4 |
| P | $p_1$ | 1.03684E-3 | 1.03791E-3 | 1.02362E-3 | 1.06543E-3 |
| | $p_2$ | -6.47852E-3 | -9.66413E-4 | 3.51079E-3 | -1.63585E-2 |
| | $p_3$ | -2.73925E-1 | -3.23738E-1 | -3.89777E-1 | -2.07133E-1 |
| | $p_4$ | 2.97735E+0 | 2.97747E+0 | 2.97478E+0 | 2.97764E+0 |
| | $\sigma$ | 1.45980E-3 | 1.26954E-3 | 2.15242E-3 | 1.25407E-3 |

Table 10. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $Cd_xZn_{1-x}Se/ZnSe$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| CdSe | | | | | |
| Cd | $p_1$ | 1.03043E-3 | 1.03842E-3 | 1.03794E-3 | 1.00666E-3 |
| | $p_2$ | -7.12259E-4 | 1.36992E-2 | -4.24217E-4 | -3.23243E-3 |
| | $p_3$ | 3.70161E-1 | 4.54750E-1 | 6.27987E-1 | 2.60507E-1 |
| | $p_4$ | 5.81898E+0 | 5.82145E+0 | 5.81886E+0 | 5.81784E+0 |
| | $\sigma$ | 1.21070E-3 | 1.14462E-3 | 1.04878E-3 | 6.25249E-4 |
| Se | $p_1$ | 1.01768E-3 | 1.04453E-3 | 1.00754E-3 | 1.01235E-3 |
| | $p_2$ | -5.55276E-3 | 4.29525E-3 | -1.50209E-2 | -6.36182E-3 |
| | $p_3$ | 3.00569E-1 | 3.54461E-1 | 4.76499E-1 | 2.27468E-1 |
| | $p_4$ | 4.38943E+0 | 4.39234E+0 | 4.39049E+0 | 4.38840E+0 |
| | $\sigma$ | 1.57060E-3 | 1.66235E-3 | 1.72828E-3 | 9.37635E-4 |
| ZnSe | | | | | |
| Zn | $p_1$ | 1.01750E-3 | 1.05800E-3 | 1.04017E-3 | 1.04421E-3 |
| | $p_2$ | 2.75732E-3 | 1.42158E-2 | 6.13410E-3 | -1.49072E-3 |
| | $p_3$ | 2.70114E-1 | 3.32891E-1 | 4.61911E-1 | 1.89519E-1 |
| | $p_4$ | 3.69467E+0 | 3.69613E+0 | 3.69423E+0 | 3.69412E+0 |
| | $\sigma$ | 1.34316E-3 | 1.24264E-3 | 1.10660E-3 | 7.65508E-4 |
| Se | $p_1$ | 1.02026E-3 | 1.04518E-3 | 1.01690E-3 | 1.01886E-3 |
| | $p_2$ | -5.54513E-3 | 3.31832E-3 | -1.37432E-2 | -5.17392E-3 |
| | $p_3$ | 2.99274E-1 | 3.54251E-1 | 4.72877E-1 | 2.24705E-1 |
| | $p_4$ | 4.43101E+0 | 4.43373E+0 | 4.43249E+0 | 4.42982E+0 |
| | $\sigma$ | 1.50608E-3 | 1.50358E-3 | 1.51598E-3 | 8.48828E-4 |

Table 11. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $Mg_xZn_{1-x}Se/ZnSe$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| MgSe | | | | | |
| Mg | $p_1$ | 9.84565E-4 | 1.02702E-3 | 1.09639E-3 | 1.04985E-3 |
| | $p_2$ | 3.71899E-4 | 2.61009E-3 | 2.64820E-2 | 8.17182E-3 |
| | $p_3$ | 1.59841E-1 | 2.06342E-1 | 2.62516E-1 | 1.01347E-1 |
| | $p_4$ | 2.11430E+0 | 2.11265E+0 | 2.11367E+0 | 2.11623E+0 |
| | $\sigma$ | 2.30116E-3 | 1.82139E-3 | 3.38551E-3 | 1.62084E-3 |
| Se | $p_1$ | 1.02606E-3 | 1.02176E-3 | 1.06034E-3 | 1.03031E-3 |
| | $p_2$ | -6.40964E-3 | -4.97706E-3 | 1.06111E-2 | 6.10705E-3 |
| | $p_3$ | 1.69585E-1 | 2.06650E-1 | 2.52714E-1 | 1.15067E-1 |
| | $p_4$ | 4.37585E+0 | 4.37506E+0 | 4.37701E+0 | 4.37752E+0 |
| | $\sigma$ | 1.17254E-3 | 6.96744E-4 | 1.63781E-3 | 8.11536E-4 |
| ZnSe | | | | | |
| Zn | $p_1$ | 1.05181E-3 | 1.05399E-3 | 1.04281E-3 | 1.03990E-3 |
| | $p_2$ | -3.32827E-3 | -7.14227E-4 | 2.20254E-2 | 8.17936E-3 |
| | $p_3$ | 1.64642E-1 | 2.09503E-1 | 2.66908E-1 | 1.00689E-1 |
| | $p_4$ | 3.69305E+0 | 3.69214E+0 | 3.69347E+0 | 3.69557E+0 |
| | $\sigma$ | 1.46760E-3 | 1.21076E-3 | 9.70151E-4 | 1.07140E-3 |
| Se | $p_1$ | 1.02212E-3 | 1.04085E-3 | 1.04563E-3 | 1.08758E-3 |
| | $p_2$ | -6.36447E-3 | -4.58594E-3 | 1.39108E-2 | 6.58852E-3 |
| | $p_3$ | 1.83880E-1 | 2.25552E-1 | 2.79017E-1 | 1.22139E-1 |
| | $p_4$ | 4.42827E+0 | 4.42785E+0 | 4.42991E+0 | 4.43073E+0 |
| | $\sigma$ | 1.27083E-3 | 8.93657E-4 | 8.02780E-4 | 9.29258E-4 |

Table 12. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $ZnS_xSe_{1-x}$/ZnSe for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| ZnS | | | | | |
| Zn | $p_1$ | 1.04749E-3 | 1.02352E-3 | 1.06526E-3 | 1.05397E-3 |
| | $p_2$ | -6.11544E-3 | 1.71660E-3 | -1.03387E-2 | -8.97796E-3 |
| | $p_3$ | -1.86235E-1 | -2.44604E-1 | -3.15253E-1 | -1.23863E-1 |
| | $p_4$ | 3.72187E+0 | 3.72323E+0 | 3.72219E+0 | 3.72126E+0 |
| | $\sigma$ | 1.12708E-3 | 9.54940E-4 | 6.16903E-4 | 7.92512E-4 |
| S | $p_1$ | 1.06030E-3 | 1.03877E-3 | 1.06477E-3 | 1.10253E-3 |
| | $p_2$ | -8.17500E-3 | -3.37458E-3 | -1.81094E-2 | -1.10122E-2 |
| | $p_3$ | -1.64251E-1 | -2.09545E-1 | -2.59668E-1 | -1.14673E-1 |
| | $p_4$ | 3.06119E+0 | 3.06329E+0 | 3.06166E+0 | 3.05960E+0 |
| | $\sigma$ | 1.32204E-3 | 1.26373E-3 | 9.10713E-4 | 9.35264E-4 |
| ZnSe | | | | | |
| Zn | $p_1$ | 1.07408E-3 | 1.02766E-3 | 1.05550E-3 | 1.12324E-3 |
| | $p_2$ | -5.27655E-3 | 2.25704E-3 | -9.80027E-3 | -8.70402E-3 |
| | $p_3$ | -1.84751E-1 | -2.42527E-1 | -3.10407E-1 | -1.22285E-1 |
| | $p_4$ | 3.69382E+0 | 3.69517E+0 | 3.69360E+0 | 3.69270E+0 |
| | $\sigma$ | 1.22320E-3 | 9.04316E-4 | 6.77333E-4 | 8.56500E-4 |
| Se | $p_1$ | 1.07168E-3 | 1.02537E-3 | 1.06100E-3 | 1.10447E-3 |
| | $p_2$ | -1.13195E-2 | -3.89573E-3 | -2.14407E-2 | -1.10812E-2 |
| | $p_3$ | -2.11772E-1 | -2.72055E-1 | -3.41937E-1 | -1.50857E-1 |
| | $p_4$ | 4.42893E+0 | 4.43107E+0 | 4.43043E+0 | 4.42807E+0 |
| | $\sigma$ | 1.11900E-3 | 1.04030E-3 | 6.54906E-4 | 7.29174E-4 |

Table 13. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $Mg_xZn_{1-x}Te/ZnTe$ ZnTeMgTe for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| MgTe | | | | | |
| Mg | $p_1$ | 1.04738E-3 | 1.02909E-3 | 1.02653E-3 | 1.09508E-3 |
| | $p_2$ | -3.09422E-4 | -7.32325E-3 | -7.03650E-3 | 5.03796E-3 |
| | $p_3$ | 2.22190E-1 | 2.76757E-1 | 3.50257E-1 | 1.56012E-1 |
| | $p_4$ | 2.26163E+0 | 2.26225E+0 | 2.26434E+0 | 2.26149E+0 |
| | $\sigma$ | 2.25216E-3 | 1.56305E-3 | 2.35278E-3 | 1.43925E-3 |
| Te | $p_1$ | 1.03440E-3 | 1.01394E-3 | 1.04497E-3 | 1.00602E-3 |
| | $p_2$ | -1.62018E-2 | -2.20795E-2 | -2.99508E-2 | 1.31076E-3 |
| | $p_3$ | 3.24096E-1 | 3.84475E-1 | 4.70581E-1 | 2.38920E-1 |
| | $p_4$ | 6.90702E+0 | 6.90879E+0 | 6.91312E+0 | 6.90664E+0 |
| | $\sigma$ | 1.19347E-3 | 8.76206E-4 | 1.50438E-3 | 5.64967E-4 |
| ZnTe | | | | | |
| Zn | $p_1$ | 1.02552E-3 | 1.01264E-3 | 1.02678E-3 | 1.02419E-3 |
| | $p_2$ | -5.57544E-3 | -1.15983E-2 | -1.17938E-2 | 2.34829E-3 |
| | $p_3$ | 2.11566E-1 | 2.62838E-1 | 3.31692E-1 | 1.46486E-1 |
| | $p_4$ | 3.84159E+0 | 3.84249E+0 | 3.84516E+0 | 3.84164E+0 |
| | $\sigma$ | 1.53905E-3 | 1.09876E-3 | 1.70166E-3 | 9.04668E-4 |
| Te | $p_1$ | 1.03670E-3 | 1.02021E-3 | 1.00661E-3 | 1.01530E-3 |
| | $p_2$ | -1.56948E-2 | -2.26420E-2 | -3.14298E-2 | 1.65940E-3 |
| | $p_3$ | 3.42199E-1 | 4.10063E-1 | 5.06401E-1 | 2.49103E-1 |
| | $p_4$ | 6.96507E+0 | 6.96660E+0 | 6.97148E+0 | 6.96414E+0 |
| | $\sigma$ | 1.27732E-3 | 8.81468E-4 | 1.58513E-3 | 5.86253E-4 |

Table 14. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $ZnS_xTe_{1-x}/ZnTe$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| ZnS | | | | | |
| Zn | $p_1$ | 1.04374E-3 | 1.04650E-3 | 1.03435E-3 | 1.06608E-3 |
| | $p_2$ | -1.74055E-2 | -3.06220E-2 | -3.60366E-2 | -1.67783E-2 |
| | $p_3$ | -4.91004E-1 | -6.09009E-1 | -8.08166E-1 | -3.34427E-1 |
| | $p_4$ | 3.94033E+0 | 3.93939E+0 | 3.94002E+0 | 3.93880E+0 |
| | $\sigma$ | 1.03825E-3 | 6.19008E-4 | 5.84523E-4 | 9.41871E-4 |
| S | $p_1$ | 1.04481E-3 | 1.02730E-3 | 1.05177E-3 | 1.09591E-3 |
| | $p_2$ | -4.40797E-2 | -6.47973E-2 | -9.88667E-2 | -2.89461E-2 |
| | $p_3$ | -3.95613E-1 | -4.82369E-1 | -6.33060E-1 | -2.85842E-1 |
| | $p_4$ | 3.25315E+0 | 3.25459E+0 | 3.26067E+0 | 3.25035E+0 |
| | $\sigma$ | 1.95253E-3 | 2.09532E-3 | 4.07455E-3 | 1.03661E-3 |
| ZnTe | | | | | |
| Zn | $p_1$ | 1.05250E-3 | 1.07289E-3 | 1.04014E-3 | 1.07556E-3 |
| | $p_2$ | -1.50049E-2 | -2.43497E-2 | -2.54285E-2 | -1.78077E-2 |
| | $p_3$ | -4.69250E-1 | -5.81471E-1 | -7.67035E-1 | -3.20060E-1 |
| | $p_4$ | 3.84043E+0 | 3.83956E+0 | 3.83941E+0 | 3.83975E+0 |
| | $\sigma$ | 1.33871E-3 | 9.98139E-4 | 1.09507E-3 | 1.14979E-3 |
| Te | $p_1$ | 1.06758E-3 | 1.05523E-3 | 9.22279E-4 | 1.06974E-3 |
| | $p_2$ | -6.16062E-2 | -9.88729E-2 | -2.39720E-1 | -4.26871E-2 |
| | $p_3$ | -8.07315E-1 | -9.90750E-1 | -1.22020E+0 | -5.68944E-1 |
| | $p_4$ | 6.96785E+0 | 6.96940E+0 | 6.96280E+0 | 6.96307E+0 |
| | $\sigma$ | 1.33980E-3 | 1.34183E-3 | 4.33071E-4 | 5.47956E-4 |

Table 15. *Table of polynomial coefficients for the 002 modified atomic scattering amplitudes of strained $ZnSe_xTe_{1-x}/ZnTe$ for different strain states s computed within LDA using 10000 k-points. All parameters are given in Å.*

| | | $s = 0.0$ | $s = 0.5$ | $s = 1.0$ | Bulk |
|---|---|---|---|---|---|
| ZnSe | | | | | |
| Zn | $p_1$ | 1.05517E-3 | 1.05496E-3 | 1.06762E-3 | 1.02198E-3 |
| | $p_2$ | -1.49618E-2 | -1.16582E-2 | -1.71084E-2 | -6.87050E-3 |
| | $p_3$ | -2.94475E-1 | -3.74901E-1 | -4.89991E-1 | -2.09305E-1 |
| | $p_4$ | 3.90669E+0 | 3.90736E+0 | 3.90683E+0 | 3.90828E+0 |
| | $\sigma$ | 1.23969E-3 | 7.76624E-4 | 9.25137E-4 | 8.05973E-4 |
| Se | $p_1$ | 1.04954E-3 | 1.06714E-3 | 1.07939E-3 | 1.05611E-3 |
| | $p_2$ | -2.79742E-2 | -2.87850E-2 | -4.52364E-2 | -1.24979E-2 |
| | $p_3$ | -3.15118E-1 | -3.93027E-1 | -5.06102E-1 | -2.36498E-1 |
| | $p_4$ | 4.67646E+0 | 4.67832E+0 | 4.67986E+0 | 4.67722E+0 |
| | $\sigma$ | 1.09044E-3 | 8.46321E-4 | 1.14353E-3 | 7.25660E-4 |
| ZnTe | | | | | |
| Zn | $p_1$ | 1.05517E-3 | 1.02520E-3 | 1.04138E-3 | 1.03137E-3 |
| | $p_2$ | -1.51619E-2 | -1.01713E-2 | -1.46415E-2 | -6.47985E-3 |
| | $p_3$ | -2.85436E-1 | -3.64491E-1 | -4.73665E-1 | -2.04416E-1 |
| | $p_4$ | 3.83928E+0 | 3.84055E+0 | 3.83939E+0 | 3.84051E+0 |
| | $\sigma$ | 1.40528E-3 | 9.06001E-4 | 1.22677E-3 | 1.05597E-3 |
| Te | $p_1$ | 1.07787E-3 | 1.06120E-3 | 1.09293E-3 | 1.02566E-3 |
| | $p_2$ | -3.41094E-2 | -3.87991E-2 | -6.11183E-2 | -1.66181E-2 |
| | $p_3$ | -4.88608E-1 | -6.07513E-1 | -7.86595E-1 | -3.57042E-1 |
| | $p_4$ | 6.96352E+0 | 6.96492E+0 | 6.96676E+0 | 6.96314E+0 |
| | $\sigma$ | 1.07256E-3 | 6.91707E-4 | 9.37796E-4 | 5.58260E-4 |

Table 16. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $GaN_xAs_{1-x}/GaAs$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Ga | N | $p_1$ | -2.43779E-1 | -3.18437E-1 | 4.12842E-2 | -1.89079E-1 |
| Ga | N | $p_2$ | 7.73953E-1 | 8.98228E-1 | 6.32657E-1 | 6.42517E-1 |
| Ga | N | $p_3$ | -4.08680E-1 | -4.62140E-1 | -4.24026E-1 | -3.29231E-1 |
| Ga | N | $p_4$ | 8.77225E-1 | 8.78236E-1 | 8.73825E-1 | 8.74055E-1 |
| Ga | As | $p_1$ | -3.53461E-1 | -3.80318E-1 | 4.68231E-1 | -2.07938E-1 |
| Ga | As | $p_2$ | 9.36571E-1 | 9.71883E-1 | 2.02269E-1 | 7.41930E-1 |
| Ga | As | $p_3$ | -7.38028E-1 | -7.54210E-1 | -5.75056E-1 | -6.47606E-1 |
| Ga | As | $p_4$ | 1.00931E+0 | 1.00851E+0 | 9.97916E-1 | 1.00388E+0 |
| N | Ga | $p_1$ | -4.52677E-1 | -6.21407E-1 | -7.45863E-1 | -3.07091E-1 |
| N | Ga | $p_2$ | 9.57547E-1 | 1.17325E+0 | 1.33522E+0 | 7.29845E-1 |
| N | Ga | $p_3$ | -5.15430E-1 | -5.73911E-1 | -6.04380E-1 | -4.29030E-1 |
| N | Ga | $p_4$ | 1.00830E+0 | 1.00997E+0 | 1.00969E+0 | 1.00337E+0 |
| As | Ga | $p_1$ | -4.86006E-1 | -6.92697E-1 | -9.63809E-1 | -2.86081E-1 |
| As | Ga | $p_2$ | 9.59107E-1 | 1.21394E+0 | 1.50060E+0 | 6.58384E-1 |
| As | Ga | $p_3$ | -4.85342E-1 | -5.49604E-1 | -6.00607E-1 | -3.78714E-1 |
| As | Ga | $p_4$ | 1.00985E+0 | 1.01161E+0 | 1.01195E+0 | 1.00372E+0 |

Table 17. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $Al_xGa_{1-x}As/GaAs$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Al | As | $p_1$ | 1.72513E-7 | 4.46276E-7 | 4.18318E-7 | -5.67096E-8 |
| Al | As | $p_2$ | 9.16947E-6 | 8.85562E-6 | 8.99871E-6 | 9.46239E-6 |
| Al | As | $p_3$ | -9.33466E-6 | -9.28356E-6 | -9.40870E-6 | -9.40634E-6 |
| Al | As | $p_4$ | 1.00000E-0 | 1.00000E-0 | 1.00000E-0 | 1.00000E+0 |
| As | Al | $p_1$ | -6.57355E-9 | 4.80856E-7 | 5.29110E-7 | -2.98324E-7 |
| As | Al | $p_2$ | 1.51650E-5 | 1.45974E-5 | 1.47939E-5 | 1.54308E-5 |
| As | Al | $p_3$ | -1.04881E-5 | -1.03758E-5 | -1.06406E-5 | -1.04687E-5 |
| As | Al | $p_4$ | 9.99995E-1 | 9.99995E-1 | 9.99995E-1 | 9.99995E-1 |
| Ga | As | $p_1$ | 1.81818E-7 | 4.15936E-7 | 4.13814E-7 | -7.24931E-8 |
| Ga | As | $p_2$ | 9.15334E-6 | 8.90682E-6 | 8.99698E-6 | 9.47617E-6 |
| Ga | As | $p_3$ | -9.32649E-6 | -9.30466E-6 | -9.40163E-6 | -9.40573E-6 |
| Ga | As | $p_4$ | 1.00000E-0 | 1.00000E-0 | 1.00000E-0 | 1.00000E+0 |
| As | Ga | $p_1$ | 1.00009E-7 | 3.90126E-7 | 6.38251E-7 | -2.22773E-7 |
| As | Ga | $p_2$ | 1.50247E-5 | 1.46714E-5 | 1.43810E-5 | 1.55082E-5 |
| As | Ga | $p_3$ | -1.97527E-5 | -1.97436E-5 | -1.97874E-5 | -1.98425E-5 |
| As | Ga | $p_4$ | 1.00000E-0 | 1.00000E-0 | 1.00000E-0 | 1.00000E+0 |

Table 18. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $GaSb_xAs_{1-x}/GaAs$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Ga | Sb | $p_1$ | 3.42761E-3 | 2.21311E-3 | 1.15464E-3 | 4.45711E-3 |
| Ga | Sb | $p_2$ | 3.84735E-2 | 3.89847E-2 | 3.90321E-2 | 3.86206E-2 |
| Ga | Sb | $p_3$ | -2.88981E-2 | -2.81873E-2 | -2.71865E-2 | -3.01041E-2 |
| Ga | Sb | $p_4$ | 9.87005E-1 | 9.86986E-1 | 9.86991E-1 | 9.87034E-1 |
| Ga | As | $p_1$ | 2.85652E-3 | 5.88538E-4 | -1.28863E-3 | 4.17954E-3 |
| Ga | As | $p_2$ | 3.73833E-2 | 4.01337E-2 | 4.22638E-2 | 3.61992E-2 |
| Ga | As | $p_3$ | -5.35736E-2 | -5.37143E-2 | -5.34926E-2 | -5.42615E-2 |
| Ga | As | $p_4$ | 9.99968E-1 | 9.99965E-1 | 9.99954E-1 | 1.00002E+0 |
| Sb | Ga | $p_1$ | 6.66422E-3 | 5.41257E-3 | 4.51688E-3 | 7.05375E-3 |
| Sb | Ga | $p_2$ | 1.59792E-2 | 1.73835E-2 | 1.83401E-2 | 1.60311E-2 |
| Sb | Ga | $p_3$ | -2.26054E-2 | -2.27724E-2 | -2.28287E-2 | -2.30977E-2 |
| Sb | Ga | $p_4$ | 9.99976E-1 | 9.99975E-1 | 9.99980E-1 | 1.00001E+0 |
| As | Ga | $p_1$ | 6.67176E-3 | 5.54273E-3 | 4.57114E-3 | 7.24007E-3 |
| As | Ga | $p_2$ | 1.74290E-2 | 1.86577E-2 | 1.96835E-2 | 1.72696E-2 |
| As | Ga | $p_3$ | -2.40763E-2 | -2.41652E-2 | -2.42262E-2 | -2.45223E-2 |
| As | Ga | $p_4$ | 9.99979E-1 | 9.99970E-1 | 9.99976E-1 | 1.00001E+0 |

Table 19. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $In_xGa_{1-x}P/GaP$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| In | P | $p_1$ | 1.10463E-2 | 1.26527E-2 | 1.51138E-2 | 9.12191E-3 |
| In | P | $p_2$ | 1.18583E-2 | 9.80301E-3 | 6.66969E-3 | 1.44881E-2 |
| In | P | $p_3$ | -2.28970E-2 | -2.24309E-2 | -2.17651E-2 | -2.36324E-2 |
| In | P | $p_4$ | 9.99973E-1 | 9.99935E-1 | 9.99895E-1 | 1.00002E+0 |
| P | In | $p_1$ | 7.97515E-3 | 1.14711E-2 | 1.58183E-2 | 4.99154E-3 |
| P | In | $p_2$ | 3.62179E-2 | 3.22005E-2 | 2.77120E-2 | 3.93718E-2 |
| P | In | $p_3$ | -3.05610E-2 | -2.99524E-2 | -2.98489E-2 | -3.07571E-2 |
| P | In | $p_4$ | 9.86336E-1 | 9.86246E-1 | 9.86242E-1 | 9.86373E-1 |
| Ga | P | $p_1$ | 1.11408E-2 | 1.29297E-2 | 1.55943E-2 | 8.93895E-3 |
| Ga | P | $p_2$ | 1.37524E-2 | 1.16148E-2 | 8.31690E-3 | 1.66047E-2 |
| Ga | P | $p_3$ | -2.48830E-2 | -2.45167E-2 | -2.38857E-2 | -2.55714E-2 |
| Ga | P | $p_4$ | 9.99965E-1 | 9.99933E-1 | 9.99893E-1 | 1.00001E+0 |
| P | Ga | $p_1$ | 5.90052E-3 | 7.18625E-3 | 9.38979E-3 | 4.24619E-3 |
| P | Ga | $p_2$ | 3.50254E-2 | 3.28009E-2 | 2.88680E-2 | 3.80139E-2 |
| P | Ga | $p_3$ | -5.59267E-2 | -5.56640E-2 | -5.49927E-2 | -5.65630E-2 |
| P | Ga | $p_4$ | 9.99957E-1 | 9.99932E-1 | 9.99891E-1 | 1.00000E+0 |

Table 20. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $GaAs_xSb_{1-x}/GaSb$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Ga | As | $p_1$ | -6.15847E-4 | 2.21885E-3 | 6.31571E-3 | -4.32525E-3 |
| Ga | As | $p_2$ | 4.52386E-2 | 4.25874E-2 | 3.87706E-2 | 4.88310E-2 |
| Ga | As | $p_3$ | -3.07377E-2 | -3.09217E-2 | -3.11198E-2 | -3.06385E-2 |
| Ga | As | $p_4$ | 9.86108E-1 | 9.86103E-1 | 9.86063E-1 | 9.86120E-1 |
| Ga | Sb | $p_1$ | -1.40136E-3 | 2.72500E-4 | 2.58912E-3 | -4.61034E-3 |
| Ga | Sb | $p_2$ | 4.73053E-2 | 4.48571E-2 | 4.12538E-2 | 5.21286E-2 |
| Ga | Sb | $p_3$ | -5.97835E-2 | -5.97798E-2 | -5.96989E-2 | -6.05270E-2 |
| Ga | Sb | $p_4$ | 9.99969E-1 | 9.99974E-1 | 9.99983E-1 | 1.00001E+0 |
| As | Ga | $p_1$ | -5.11153E-3 | -3.61911E-3 | -2.00915E-3 | -7.36718E-3 |
| As | Ga | $p_2$ | 3.64035E-2 | 3.48578E-2 | 3.33647E-2 | 3.91041E-2 |
| As | Ga | $p_3$ | -3.12711E-2 | -3.12082E-2 | -3.12770E-2 | -3.17564E-2 |
| As | Ga | $p_4$ | 9.99981E-1 | 9.99983E-1 | 9.99993E-1 | 1.00001E+0 |
| Sb | Ga | $p_1$ | -5.05189E-3 | -3.54090E-3 | -1.91399E-3 | -7.25463E-3 |
| Sb | Ga | $p_2$ | 3.47780E-2 | 3.32186E-2 | 3.16616E-2 | 3.74214E-2 |
| Sb | Ga | $p_3$ | -2.97133E-2 | -2.96403E-2 | -2.96694E-2 | -3.01946E-2 |
| Sb | Ga | $p_4$ | 9.99984E-1 | 9.99981E-1 | 9.99995E-1 | 1.00001E+0 |

Table 21. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $Ga_xIn_{1-x}P/InP$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Ga | P | $p_1$ | -9.12092E-3 | -8.87471E-3 | -9.66072E-3 | -8.31048E-3 |
| Ga | P | $p_2$ | 4.30754E-2 | 4.23877E-2 | 4.31007E-2 | 4.24842E-2 |
| Ga | P | $p_3$ | -3.39409E-2 | -3.34504E-2 | -3.33836E-2 | -3.41433E-2 |
| Ga | P | $p_4$ | 9.99974E-1 | 9.99940E-1 | 9.99935E-1 | 9.99984E-1 |
| P | Ga | $p_1$ | -4.45960E-3 | -3.57403E-3 | -4.13163E-3 | -3.59181E-3 |
| P | Ga | $p_2$ | 4.97835E-2 | 4.76109E-2 | 4.74027E-2 | 4.97418E-2 |
| P | Ga | $p_3$ | -3.10407E-2 | -2.96480E-2 | -2.89187E-2 | -3.18424E-2 |
| P | Ga | $p_4$ | 9.85692E-1 | 9.85614E-1 | 9.85642E-1 | 9.85697E-1 |
| In | P | $p_1$ | -8.51779E-3 | -8.03325E-3 | -7.97711E-3 | -8.47278E-3 |
| In | P | $p_2$ | 4.05747E-2 | 3.97303E-2 | 3.94710E-2 | 4.08359E-2 |
| In | P | $p_3$ | -3.20383E-2 | -3.16388E-2 | -3.14375E-2 | -3.23361E-2 |
| In | P | $p_4$ | 9.99975E-1 | 9.99949E-1 | 9.99933E-1 | 9.99992E-1 |
| P | In | $p_1$ | -6.62109E-3 | -7.47700E-3 | -9.02474E-3 | -4.34485E-3 |
| P | In | $p_2$ | 5.57888E-2 | 5.65217E-2 | 5.80451E-2 | 5.33652E-2 |
| P | In | $p_3$ | -6.24762E-2 | -6.21148E-2 | -6.17583E-2 | -6.26217E-2 |
| P | In | $p_4$ | 9.99966E-1 | 9.99942E-1 | 9.99918E-1 | 9.99978E-1 |

Table 22. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $Cd_xZn_{1-x}Se/ZnSe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Cd | Se | $p_1$ | 2.74614E-3 | 2.19777E-3 | 1.99605E-4 | 4.12846E-3 |
| Cd | Se | $p_2$ | 2.28091E-2 | 2.31686E-2 | 2.52659E-2 | 2.15635E-2 |
| Cd | Se | $p_3$ | -2.55453E-2 | -2.53186E-2 | -2.54281E-2 | -2.56887E-2 |
| Cd | Se | $p_4$ | 9.99989E-1 | 9.99971E-1 | 9.99972E-1 | 1.00000E+0 |
| Se | Cd | $p_1$ | -1.41199E-3 | -1.70957E-3 | -3.99397E-3 | 4.29444E-4 |
| Se | Cd | $p_2$ | 4.29905E-2 | 4.20191E-2 | 4.33049E-2 | 4.21218E-2 |
| Se | Cd | $p_3$ | -2.80449E-2 | -2.66724E-2 | -2.57143E-2 | -2.90197E-2 |
| Se | Cd | $p_4$ | 9.86446E-1 | 9.86373E-1 | 9.86396E-1 | 9.86462E-1 |
| Zn | Se | $p_1$ | 2.72912E-3 | 2.11133E-3 | 1.51032E-4 | 4.04547E-3 |
| Zn | Se | $p_2$ | 2.36610E-2 | 2.41357E-2 | 2.61273E-2 | 2.24909E-2 |
| Zn | Se | $p_3$ | -2.63778E-2 | -2.61975E-2 | -2.62377E-2 | -2.65379E-2 |
| Zn | Se | $p_4$ | 9.99987E-1 | 9.99971E-1 | 9.99966E-1 | 1.00000E-0 |
| Se | Zn | $p_1$ | -2.81979E-3 | -4.08009E-3 | -6.64130E-3 | -7.02337E-4 |
| Se | Zn | $p_2$ | 4.71045E-2 | 4.85800E-2 | 5.15016E-2 | 4.47356E-2 |
| Se | Zn | $p_3$ | -5.64000E-2 | -5.61335E-2 | -5.58300E-2 | -5.67249E-2 |
| Se | Zn | $p_4$ | 9.99963E-1 | 9.99945E-1 | 9.99923E-1 | 9.99987E-1 |

Table 23. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $Mg_xZn_{1-x}Se/ZnSe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Mg | Se | $p_1$ | 3.66248E-3 | 4.34810E-3 | 5.33168E-3 | 3.01994E-3 |
| Mg | Se | $p_2$ | 4.98440E-3 | 4.05649E-3 | 2.71941E-3 | 5.92234E-3 |
| Mg | Se | $p_3$ | -8.65912E-3 | -8.40463E-3 | -8.07532E-3 | -8.96015E-3 |
| Mg | Se | $p_4$ | 9.99993E-1 | 9.99975E-1 | 9.99956E-1 | 1.00001E+0 |
| Se | Mg | $p_1$ | 3.91969E-3 | 5.57046E-3 | 7.81594E-3 | 2.56406E-3 |
| Se | Mg | $p_2$ | 1.14122E-2 | 9.47417E-3 | 7.03523E-3 | 1.29167E-2 |
| Se | Mg | $p_3$ | -1.08916E-2 | -1.05686E-2 | -1.04095E-2 | -1.10454E-2 |
| Se | Mg | $p_4$ | 9.95542E-1 | 9.95506E-1 | 9.95498E-1 | 9.95560E-1 |
| Zn | Se | $p_1$ | 4.13892E-3 | 4.97634E-3 | 6.12573E-3 | 3.31615E-3 |
| Zn | Se | $p_2$ | 4.87663E-3 | 3.82505E-3 | 2.35139E-3 | 5.97669E-3 |
| Zn | Se | $p_3$ | -9.02712E-3 | -8.79988E-3 | -8.49886E-3 | -9.31307E-3 |
| Zn | Se | $p_4$ | 9.99990E-1 | 9.99974E-1 | 9.99957E-1 | 1.00001E+0 |
| Se | Zn | $p_1$ | 3.52800E-3 | 4.10778E-3 | 4.88956E-3 | 2.99877E-3 |
| Se | Zn | $p_2$ | 1.01395E-2 | 9.05524E-3 | 7.36650E-3 | 1.12690E-2 |
| Se | Zn | $p_3$ | -1.90425E-2 | -1.88699E-2 | -1.85925E-2 | -1.92856E-2 |
| Se | Zn | $p_4$ | 9.99996E-1 | 9.99983E-1 | 9.99967E-1 | 1.00001E+0 |

Table 24. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $ZnS_xSe_{1-x}/ZnSe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Zn | S | $p_1$ | 2.93747E-3 | 5.03443E-3 | 8.44638E-3 | 1.32293E-3 |
| Zn | S | $p_2$ | 1.98900E-2 | 1.79668E-2 | 1.46380E-2 | 2.11400E-2 |
| Zn | S | $p_3$ | -1.62903E-2 | -1.64416E-2 | -1.65188E-2 | -1.59244E-2 |
| Zn | S | $p_4$ | 9.93454E-1 | 9.93433E-1 | 9.93409E-1 | 9.93469E-1 |
| Zn | Se | $p_1$ | 2.17557E-3 | 4.15031E-3 | 6.91250E-3 | 9.98035E-4 |
| Zn | Se | $p_2$ | 1.91514E-2 | 1.64584E-2 | 1.23612E-2 | 2.08953E-2 |
| Zn | Se | $p_3$ | -2.90048E-2 | -2.87746E-2 | -2.83224E-2 | -2.89839E-2 |
| Zn | Se | $p_4$ | 1.00001E+0 | 9.99994E-1 | 9.99971E-1 | 1.00001E+0 |
| S | Zn | $p_1$ | 3.21228E-4 | 1.61253E-3 | 3.45398E-3 | -6.15692E-4 |
| S | Zn | $p_2$ | 1.48663E-2 | 1.35131E-2 | 1.13857E-2 | 1.58659E-2 |
| S | Zn | $p_3$ | -1.51906E-2 | -1.51200E-2 | -1.48388E-2 | -1.52602E-2 |
| S | Zn | $p_4$ | 1.00000E+0 | 1.00000E+0 | 9.99991E-1 | 1.00002E+0 |
| Se | Zn | $p_1$ | 4.45760E-4 | 1.64373E-3 | 3.50932E-3 | -4.85727E-4 |
| Se | Zn | $p_2$ | 1.45132E-2 | 1.32578E-2 | 1.11173E-2 | 1.55039E-2 |
| Se | Zn | $p_3$ | -1.49608E-2 | -1.49007E-2 | -1.46220E-2 | -1.50267E-2 |
| Se | Zn | $p_4$ | 1.00000E+0 | 1.00000E+0 | 9.99989E-1 | 1.00002E+0 |

Table 25. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $Mg_xZn_{1-x}Te/ZnTe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Mg | Te | $p_1$ | -5.42302E-4 | -1.54754E-3 | -3.15861E-3 | 1.18299E-3 |
| Mg | Te | $p_2$ | 1.40799E-2 | 1.50143E-2 | 1.64450E-2 | 1.24184E-2 |
| Mg | Te | $p_3$ | -1.35361E-2 | -1.34490E-2 | -1.32718E-2 | -1.35946E-2 |
| Mg | Te | $p_4$ | 1.00000E+0 | 9.99996E-1 | 9.99985E-1 | 1.00001E+0 |
| Te | Mg | $p_1$ | -2.15337E-3 | -3.46925E-3 | -5.58208E-3 | 4.07003E-4 |
| Te | Mg | $p_2$ | 2.37199E-2 | 2.40023E-2 | 2.46920E-2 | 2.21611E-2 |
| Te | Mg | $p_3$ | -1.47825E-2 | -1.37015E-2 | -1.22954E-2 | -1.57768E-2 |
| Te | Mg | $p_4$ | 9.93218E-1 | 9.93183E-1 | 9.93179E-1 | 9.93228E-1 |
| Zn | Te | $p_1$ | -3.11074E-4 | -1.38667E-3 | -3.00167E-3 | 1.41553E-3 |
| Zn | Te | $p_2$ | 1.39619E-2 | 1.50031E-2 | 1.64102E-2 | 1.22947E-2 |
| Zn | Te | $p_3$ | -1.36477E-2 | -1.35991E-2 | -1.33931E-2 | -1.37058E-2 |
| Zn | Te | $p_4$ | 1.00000E+0 | 9.99998E-1 | 9.99984E-1 | 1.00001E+0 |
| Te | Zn | $p_1$ | -2.10395E-3 | -3.96383E-3 | -6.49367E-3 | 5.69181E-4 |
| Te | Zn | $p_2$ | 2.49149E-2 | 2.72363E-2 | 3.00444E-2 | 2.16565E-2 |
| Te | Zn | $p_3$ | -2.88361E-2 | -2.87113E-2 | -2.82296E-2 | -2.90100E-2 |
| Te | Zn | $p_4$ | 1.00000E-0 | 9.99993E-1 | 9.99965E-1 | 1.00001E+0 |

Table 26. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $ZnS_xTe_{1-x}/ZnTe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Zn | S | $p_1$ | 4.84295E-2 | 8.06254E-2 | 1.40525E-1 | 1.44536E-2 |
| Zn | S | $p_2$ | 8.89816E-2 | 5.55117E-2 | -5.60181E-3 | 1.23644E-1 |
| Zn | S | $p_3$ | -9.60974E-2 | -9.49173E-2 | -9.40123E-2 | -9.68683E-2 |
| Zn | S | $p_4$ | 9.58190E-1 | 9.57893E-1 | 9.57426E-1 | 9.58666E-1 |
| Zn | Te | $p_1$ | 2.72196E-2 | 4.52461E-2 | 7.47365E-2 | 1.58324E-3 |
| Zn | Te | $p_2$ | 9.56530E-2 | 6.56234E-2 | 1.50752E-2 | 1.36142E-1 |
| Zn | Te | $p_3$ | -1.79306E-1 | -1.76806E-1 | -1.74402E-1 | -1.84863E-1 |
| Zn | Te | $p_4$ | 9.99463E-1 | 9.99357E-1 | 9.99263E-1 | 9.99900E-1 |
| S | Zn | $p_1$ | 3.22509E-3 | 2.09692E-2 | 5.12864E-2 | -1.73808E-2 |
| S | Zn | $p_2$ | 9.80071E-2 | 7.76496E-2 | 4.59476E-2 | 1.22706E-1 |
| S | Zn | $p_3$ | -1.00916E-1 | -9.82947E-2 | -9.70241E-2 | -1.05249E-1 |
| S | Zn | $p_4$ | 9.99572E-1 | 9.99464E-1 | 9.99441E-1 | 9.99937E-1 |
| Te | Zn | $p_1$ | 3.73735E-3 | 2.09395E-2 | 4.86909E-2 | -1.50974E-2 |
| Te | Zn | $p_2$ | 9.22962E-2 | 7.25046E-2 | 4.39847E-2 | 1.14875E-1 |
| Te | Zn | $p_3$ | -9.57659E-2 | -9.30888E-2 | -9.24336E-2 | -9.96960E-2 |
| Te | Zn | $p_4$ | 9.99594E-1 | 9.99461E-1 | 9.99478E-1 | 9.99930E-1 |

Table 27. *Table of polynomial coefficients for the static displacement correction factors $d^{002}_{A,B}$ to the 002 SF of strained $ZnSe_xTe_{1-x}/ZnTe$, with A the atom considered and B its nearest neighbor.*

| A | B | | $s$=0.0 | $s$=0.5 | $s$=1.0 | Bulk |
|---|---|---|---|---|---|---|
| Zn | Se | $p_1$ | 7.01944E-3 | 1.11827E-2 | 2.26863E-2 | 8.12887E-4 |
| Zn | Se | $p_2$ | 4.69320E-2 | 4.40792E-2 | 3.20655E-2 | 5.26260E-2 |
| Zn | Se | $p_3$ | -3.82260E-2 | -3.95521E-2 | -3.90033E-2 | -3.77357E-2 |
| Zn | Se | $p_4$ | 9.84239E-1 | 9.84276E-1 | 9.84103E-1 | 9.84294E-1 |
| Zn | Te | $p_1$ | 5.01801E-3 | 7.34759E-3 | 1.52551E-2 | -6.33143E-4 |
| Zn | Te | $p_2$ | 4.57830E-2 | 4.26338E-2 | 3.03033E-2 | 5.41012E-2 |
| Zn | Te | $p_3$ | -6.91446E-2 | -6.99343E-2 | -6.84246E-2 | -7.01301E-2 |
| Zn | Te | $p_4$ | 9.99965E-1 | 1.00003E+0 | 9.99903E-1 | 1.00004E+0 |
| Se | Zn | $p_1$ | -1.36370E-3 | 3.68594E-4 | 6.87043E-3 | -5.36774E-3 |
| Se | Zn | $p_2$ | 3.87260E-2 | 3.76768E-2 | 3.00203E-2 | 4.33605E-2 |
| Se | Zn | $p_3$ | -3.73493E-2 | -3.80422E-2 | -3.68696E-2 | -3.80360E-2 |
| Se | Zn | $p_4$ | 9.99992E-1 | 1.00005E+0 | 9.99942E-1 | 1.00005E+0 |
| Te | Zn | $p_1$ | -1.37583E-3 | 3.05784E-4 | 6.61551E-3 | -5.06078E-3 |
| Te | Zn | $p_2$ | 3.75192E-2 | 3.65474E-2 | 2.90564E-2 | 4.17663E-2 |
| Te | Zn | $p_3$ | -3.61445E-2 | -3.68386E-2 | -3.56481E-2 | -3.67447E-2 |
| Te | Zn | $p_4$ | 9.99997E-1 | 1.00005E+0 | 9.99940E-1 | 1.00004E+0 |