

1. Resultados: Método de deformación unidireccional

NOTA: Todos los componentes del tensor de tensiones están dados en eV/Å³.

Dirección: $\varepsilon = (\varepsilon_0, 0, 0, 0, 0, 0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.030269 | -0.009742 | -0.006796 | 0.000016 | 0.000041 | -0.007552 |
| | -0.03 | -0.021715 | -0.006763 | -0.004875 | 0.000040 | 0.000064 | -0.005685 |
| | -0.02 | -0.014990 | -0.004340 | -0.003087 | 0.000017 | 0.000003 | -0.003563 |
| | -0.01 | -0.007197 | -0.001999 | -0.001431 | 0.000015 | 0.000005 | -0.001828 |
| | 0.01 | 0.006560 | 0.002009 | 0.001612 | 0.000013 | 0.000004 | 0.001605 |
| | 0.02 | 0.012611 | 0.003814 | 0.003012 | 0.000036 | 0.000038 | 0.003182 |
| | 0.03 | 0.017913 | 0.005512 | 0.004675 | 0.000038 | 0.000011 | 0.004671 |
| | 0.04 | 0.022690 | 0.007073 | 0.005787 | 0.000010 | -0.000042 | 0.006239 |
| LDA | -0.03 | -0.025848 | -0.008938 | -0.004467 | 0.000654 | 0.000805 | -0.005197 |
| | -0.02 | -0.017147 | -0.005757 | -0.002897 | 0.000301 | 0.000598 | -0.003322 |
| | -0.01 | -0.008693 | -0.002780 | -0.001639 | 0.000151 | 0.000312 | -0.001614 |
| | 0.01 | 0.008069 | 0.002739 | 0.001355 | 0.000034 | -0.000164 | 0.001491 |
| | 0.02 | 0.014955 | 0.005417 | 0.002595 | 0.000026 | -0.000224 | 0.003092 |
| | 0.03 | 0.021623 | 0.007719 | 0.003968 | 0.000060 | -0.000345 | 0.004650 |

Dirección: $\varepsilon = (0, \varepsilon_0, 0, 0, 0, 0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.012123 | -0.033228 | -0.011473 | 0.000082 | -0.000026 | 0.011747 |
| | -0.03 | -0.008576 | -0.023903 | -0.008522 | 0.000042 | -0.000024 | 0.008491 |
| | -0.02 | -0.006197 | -0.017445 | -0.005959 | 0.000002 | -0.000001 | 0.005868 |
| | -0.01 | -0.003515 | -0.008908 | -0.003263 | 0.000009 | 0.000008 | 0.002749 |
| | 0.01 | 0.003066 | 0.008222 | 0.003039 | 0.000041 | 0.000023 | -0.002898 |
| | 0.02 | 0.005335 | 0.014466 | 0.005837 | -0.000012 | 0.000014 | -0.005686 |
| | 0.03 | 0.007471 | 0.020251 | 0.008516 | -0.000008 | 0.000007 | -0.008280 |
| | 0.04 | 0.009560 | 0.023619 | 0.012210 | 0.000060 | 0.000006 | -0.011035 |
| LDA | -0.03 | -0.009268 | -0.028657 | -0.006753 | 0.000049 | -0.000802 | 0.004789 |
| | -0.02 | -0.006364 | -0.019192 | -0.004621 | -0.000278 | -0.000514 | 0.003428 |
| | -0.01 | -0.003166 | -0.009561 | -0.002459 | 0.000050 | -0.000260 | 0.001780 |
| | 0.01 | 0.002813 | 0.009321 | 0.002345 | 0.000185 | 0.000377 | -0.001968 |
| | 0.02 | 0.005508 | 0.017940 | 0.004591 | 0.000295 | 0.000598 | -0.003911 |
| | 0.03 | 0.007937 | 0.025907 | 0.006789 | 0.000339 | 0.000895 | -0.005782 |

Dirección: $\varepsilon = (0, 0, \varepsilon_0, 0, 0, 0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.008802 | -0.010814 | -0.035824 | 0.000058 | 0.000049 | 0.002198 |
| | -0.03 | -0.006105 | -0.007534 | -0.025554 | 0.000028 | 0.000035 | 0.001533 |
| | -0.02 | -0.004527 | -0.005265 | -0.017932 | 0.000030 | 0.000054 | 0.001262 |
| | -0.01 | -0.002032 | -0.002467 | -0.008640 | 0.000035 | 0.000036 | 0.000590 |
| | 0.01 | 0.002317 | 0.002826 | 0.008828 | 0.000003 | 0.000020 | -0.000659 |
| | 0.02 | 0.003736 | 0.005072 | 0.016058 | 0.000020 | -0.000028 | -0.001399 |
| | 0.03 | 0.005429 | 0.007366 | 0.022994 | 0.000015 | 0.000002 | -0.001969 |
| | 0.04 | 0.006981 | 0.009590 | 0.029767 | -0.000003 | -0.000012 | -0.002757 |
| LDA | -0.03 | -0.002978 | -0.004888 | -0.014989 | 0.000762 | -0.001287 | 0.000204 |
| | -0.02 | -0.003105 | -0.004036 | -0.013262 | -0.000516 | -0.001004 | 0.000520 |
| | -0.01 | -0.001835 | -0.002059 | -0.007376 | -0.000562 | -0.000822 | 0.000327 |
| | 0.01 | 0.001581 | 0.002221 | 0.007334 | 0.000775 | 0.000962 | -0.000411 |
| | 0.02 | 0.003318 | 0.004186 | 0.012496 | 0.001165 | 0.001307 | -0.000728 |
| | 0.03 | 0.005348 | 0.005947 | 0.019082 | 0.002286 | 0.002050 | -0.001106 |

Dirección: $\varepsilon = (0, 0, 0, \varepsilon_0, 0, 0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.000386 | 0.000223 | -0.000979 | -0.010102 | 0.002716 | -0.000459 |
| | -0.03 | -0.000242 | 0.000201 | -0.000482 | -0.007517 | 0.001984 | -0.000321 |
| | -0.02 | -0.000196 | 0.000045 | -0.000250 | -0.006070 | 0.001912 | -0.000138 |
| | -0.01 | -0.000148 | 0.000047 | -0.000127 | -0.003358 | 0.000844 | -0.000090 |
| | 0.01 | -0.000165 | 0.000042 | -0.000088 | 0.003173 | -0.000794 | -0.000114 |
| | 0.02 | -0.000211 | 0.000045 | -0.000278 | 0.006102 | -0.001886 | -0.000160 |
| | 0.03 | -0.000228 | 0.000218 | -0.000501 | 0.007621 | -0.001966 | -0.000354 |
| | 0.04 | -0.000376 | 0.000217 | -0.000984 | 0.010224 | -0.002703 | -0.000488 |
| LDA | -0.03 | 0.000665 | 0.000805 | 0.001016 | -0.006142 | 0.002465 | 0.000615 |
| | -0.02 | 0.000212 | 0.000297 | 0.000221 | -0.004508 | 0.001672 | 0.000575 |
| | -0.01 | 0.000123 | 0.000200 | 0.000070 | -0.002458 | 0.000910 | 0.000303 |
| | 0.01 | -0.000160 | 0.000054 | -0.000210 | 0.002728 | -0.000787 | -0.000365 |
| | 0.02 | -0.000364 | 0.000088 | -0.000301 | 0.004994 | -0.001436 | -0.000852 |
| | 0.03 | -0.000765 | 0.000140 | -0.000744 | 0.007323 | -0.002089 | -0.001193 |

Dirección: $\varepsilon = (0, 0, 0, 0, \varepsilon_0, 0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.000406 | -0.000282 | -0.001244 | -0.003418 | -0.004732 | 0.000024 |
| | -0.03 | -0.000195 | -0.000098 | -0.000693 | -0.002651 | -0.003820 | -0.000045 |
| | -0.02 | -0.000173 | -0.000028 | -0.000100 | -0.001713 | -0.002624 | -0.000035 |
| | -0.01 | -0.000142 | 0.000039 | -0.000118 | -0.001131 | -0.001815 | -0.000090 |
| | 0.01 | -0.000146 | 0.000026 | -0.000137 | 0.001128 | 0.001856 | -0.000102 |
| | 0.02 | -0.000221 | -0.000050 | -0.000161 | 0.001768 | 0.002623 | -0.000073 |
| | 0.03 | -0.000240 | -0.000136 | -0.000761 | 0.002698 | 0.003863 | -0.000065 |
| | 0.04 | -0.000505 | -0.000354 | -0.001393 | 0.003423 | 0.004708 | -0.000054 |
| LDA | -0.03 | 0.000578 | 0.000538 | 0.000207 | -0.001370 | -0.002819 | 0.000742 |
| | -0.02 | 0.000312 | 0.000362 | -0.000101 | -0.001092 | -0.002129 | 0.000407 |
| | -0.01 | -0.000024 | 0.000122 | -0.000223 | -0.000577 | -0.001098 | 0.000175 |
| | 0.01 | -0.000223 | -0.000088 | -0.000003 | 0.000876 | 0.001343 | -0.000160 |
| | 0.02 | -0.000343 | -0.000171 | -0.000060 | 0.001500 | 0.002445 | -0.000420 |
| | 0.03 | -0.000513 | -0.000285 | -0.000350 | 0.002144 | 0.003411 | -0.000526 |

Dirección: $\varepsilon = (0, 0, 0, 0, 0, \varepsilon_0)$

| | ε_0 | σ_1 | σ_2 | σ_3 | σ_4 | σ_5 | σ_6 |
|-----|-----------------|------------|------------|------------|------------|------------|------------|
| GGA | -0.04 | -0.007206 | -0.016126 | -0.004239 | 0.000070 | 0.000035 | -0.009282 |
| | -0.03 | -0.004923 | -0.013252 | -0.002954 | 0.000040 | 0.000023 | -0.006846 |
| | -0.02 | -0.003051 | -0.008401 | -0.002173 | 0.000036 | 0.000022 | -0.004726 |
| | -0.01 | -0.001686 | -0.004345 | -0.000788 | 0.000021 | 0.000024 | -0.002352 |
| | 0.01 | 0.001349 | 0.004025 | 0.000601 | -0.000011 | 0.000019 | 0.002311 |
| | 0.02 | 0.002864 | 0.007232 | 0.002145 | -0.000012 | -0.000046 | 0.004194 |
| | 0.03 | 0.004071 | 0.009512 | 0.003032 | -0.000014 | -0.000056 | 0.006094 |
| | 0.04 | 0.006052 | 0.011415 | 0.004627 | -0.000048 | -0.000092 | 0.007799 |
| LDA | -0.03 | -0.005437 | -0.019124 | -0.003337 | 0.002187 | 0.000117 | -0.008610 |
| | -0.02 | -0.003360 | -0.012339 | -0.001962 | 0.001515 | 0.000127 | -0.005859 |
| | -0.01 | -0.001700 | -0.006014 | -0.001005 | 0.000793 | 0.000088 | -0.002971 |
| | 0.01 | 0.001363 | 0.005788 | 0.000951 | -0.000503 | 0.000105 | 0.002824 |
| | 0.02 | 0.002808 | 0.010857 | 0.001722 | -0.001014 | 0.000071 | 0.005607 |
| | 0.03 | 0.004464 | 0.015421 | 0.002329 | -0.001380 | 0.000212 | 0.008069 |