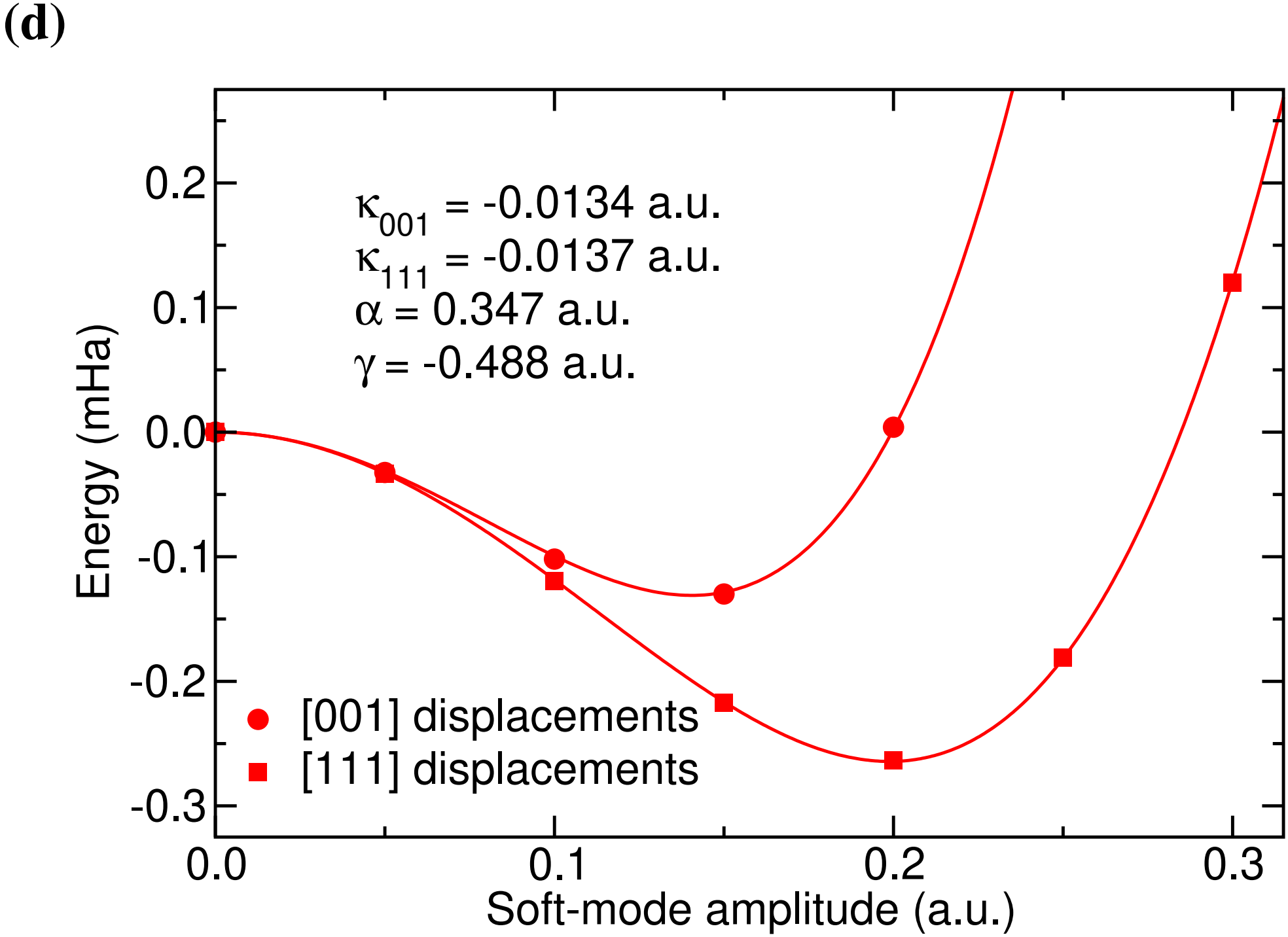
(d)
κ_{001} = -0.0134 a.u.
κ_{111} = -0.0137 a.u.
α = 0.347 a.u.
γ = -0.488 a.u.
[001] displacements
[111] displacements
Energy (mHa)
Soft-mode amplitude (a.u.)
0.2
0.1
0.0
-0.1
-0.2
-0.3
0.0
0.1
0.2
0.3