I f S -O Eff -B S

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quantum wells of realistic dimensions and concentration x. We find that the linear and the quadratic piezoelectric coefficients have the opposite effect on the field, and for large strains (large In concentration) the quadratic terms even dominate. Thus, the piezoelectric field turns out to be a rare example of a physical quantity for

and $B_{\mu jk}$ from first-principles calculations in a manner described next.

First-principles calculation of linear and nonlinear piezoelectric coefficients.—Symmetry considerations for the zinc-blende crystal structure imply that the only nonzero elements of the piezoelectric tensor are e[redacted] $=$ e[redacted] $=$ e[redacted] (i.e., there is only one independent element). Similar considerations guarantee that there are only 24 nonzero elements of the $B_{\mu jk}$

/) and neglecting the second-
Eq. (1) (triangular symbols in Fig. 3),
to the experimental procedure that
mation of e by 35%, we find for the
n of ≃ – , an overestimation of
e field by 34%–52%. Our results there-
origin of the experimentally observed
8,20,28]: A linear interpolation between
GaAs values of e cannot reproduce the
eld of alloyed quantum wells since the field
nate from the linear coefficient alone but has
ntributions from the second-order piezoelec-
$B_{\mu jk}$ (neglected in the analysis of the experi-
lts).

hasize the effect of the nonlinear tensors $B_{\mu jk}$
e plot using square symbols in Fig. 3 the piezo-
field with $e_{\mu j}$ set to the DFT values and $B_{\mu ij}$ set to
he results show that, when taking only the linear
into account, the field is overestimated by about
% in the region of low concentration [Fig. 3(b)] and
n has the wrong sign at higher concentrations.

In summary, we have shown that the second-order piezo-
ectric tensor, generally neglected so far in theoretical and
xperimental work, contributes significantly to the piezo-
electric effect in zinc-blende semiconductors. We showed
hat the piezoelectric field calculated by including first-
and second-order piezoelectric tensors obtained from DFT agree well with experiments, whereas neglect of nonlinearities leads to qualitative disagreements. We argue that the ‘‘piezoelectric coefficients’’ that have been extracted from experimental work so far are actually effective ones reflecting equally strong first- and second-order contributions.

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