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Phonon frequencies and eigendisplacements in cubic SiC and GaAs

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Abstract. An optimization procedure for determining the force constant parameters of a simple 'eleven-parameter' rigid-ion model (RIM) has been developed that yields good predictive power for the eigendisplacements (EDs). The disregard that the RIM has fallen into in the last few decades is undeserved, and here we show that given an appropriately optimized set of parameters the RIM can predict good results. The optimization procedure is presented and applied here to SiC and GaAs. For SiC the optimized parameters not only give calculated phonon frequencies which agree with the measurements to better than 6% but also predict the EDs which agree with the *ab initio* (LDF) method to better than 1%. In the case of GaAs the RIM, using the optimized parameters, predicts the observed EDs to well within the quoted experimental uncertainties. Where the measurements do not exist, the predicted EDs in GaAs agree with those calculated by the LDF method to better than 1%. As is the case for the LDF method calculations on GaAs, the present RIM calculations for the transverse acoustic (TA) frequencies show large variations from the measured values towards the zone boundaries. This implies that short-range forces from further neighbours need to be taken into account if the calculated frequencies are also to agree with the measurements. The RIM calculations presented here of EDs in SiC and GaAs using the set of force constant parameters optimized for that purpose, suggest that these calculations are essentially model independent.

1. Introduction

This paper is concerned with the prediction of eigendisplacements from other measured phonon properties. In this work we develop a novel optimization procedure for determining the force constant parameters of the RIM when it is to be used for eigendisplacement predictions. Note that our earlier parameter optimization procedures [1–3] are still valid if the sole requirement is for good eigenvalue predictions.

The reliability of the predictions of phonon frequencies in a number of compounds that crystallize with the zincblende-type structure (ZBS) on the basis of an eleven parameter RIM (11RIM) was last reassessed during 1981 by Patel *et al* [1]. A procedure for determining the optimized force constant parameters that are needed if this model is to be used for eigenvalue predictions was then developed. The use of an optimized set of force constant parameters within this model was shown at the time to improve the quality of the fits to available measured neutron scattering data. Not only were these fits better than those reported by users of non-optimized RIMs, but also the

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fits gave similar, if not better, results than calculations using the 14-parameter shell model or any of its modifications.

In the past three decades, the calculations of phonon dispersion curves and other related properties of ZBS compounds, using a number of established models, have been compared with the available measured data. Although the eigenvectors in these compounds could have been calculated on the basis of these models, experimentally there was nothing with which to compare them, since the experimental determination of eigenvectors is difficult. A number of models as well as the LDF method [4] were established by 1981. The parameters used within all of these mathematical models could be optimized to give reasonable fits to measured phonon frequencies, but they showed significantly different associated eigenvectors. This is not surprising since it was shown in 1971 by Leigh *et al* [5] 'that the force constants of a solid cannot be deduced from the lattice frequencies alone. The fact that a set of force constants agrees with the frequencies exactly is no guarantee that the force constants are even approximately correct.' In other words the force constants of a solid cannot be determined unambiguously without considering the eigendisplacements.

In 1986, the first few measurements of the eigenvectors in GaAs were reported [6], and it became possible to cross-check the reliability of the model predictions of eigenvectors in GaAs. In that 1986 cross-check [6] many models were included, but *not* our 1982 [1] or 1984 [2,3] optimized RIM. This allowed the authors of [6] to incorrectly conclude that RIM was unreliable for the predictions of eigenvectors. In a recent paper [7] we predicted the EDs in GaAs using the optimized set of force constant parameters obtained in 1982–84 [1–3] for the RIM. We found that the RIM predictions agreed well with the measured values of the EDs of the longitudinal optic (LO) and longitudinal acoustic (LA) modes at the X-point.

The measurements of EDs in TO(X) and TA(X) have not been made so far but they have been calculated by the LDF method [4]. However, the LDF method predicted phonon frequencies of these modes that compared poorly with the measurements. Since eigenvector and eigenvalue predictions are closely interrelated, it was thought that the disagreement between the predictions of the RIM and the LDF method for the EDs in the TO(X) and TA(X) modes arose simply from the poor phonon frequency predictions of the LDF method. However, it is becoming apparent that, as currently used, the LDF method seeks convergence of calculated EDs rather than convergence of the zone boundary phonon frequencies. Therefore we have attempted to reassess the optimization procedure for the RIM. We propose that if our prime interest is in predicting eigenvectors, then the appropriate optimization procedure for the model parameters should be almost entirely based on long-wavelength phonon properties. (Note that if we seek to use the RIM to predict full sets of phonon dispersion curves, without regard to EDs then our earlier optimization procedures [1–3] are still to be preferred.)

11RIM and 3RIM (a limited model) are introduced and procedures established to determine the force constant parameters, taking account of the limitations of the models and thus giving particular weight to phonon properties at long wavelengths. In this approach we propose that the dominant force constants can be determined from zone centre frequencies and the elastic constants. 3RIM is the first-order model which utilizes only the two first nearest-neighbour, force constant parameters and the static ionic charge. 11RIM is the model using force constants out to second nearest neighbours but includes the three parameters as determined by 3RIM. We show that 3RIM gives reasonable predictions of the EDs and that 11RIM (optimized as previously)

provides improved predictions. In the long-wavelength limit we expect that a simple harmonic model applies to a reasonably harmonic solid so that neglect of everything but the first-order parameters is not an unreasonable first approximation. In the calculation of the EDs the first nearest-neighbour parameters provide the dominant contribution. The contention is then that the first nearest-neighbour parameters determined by 3RIM provide a realistic description of the physical interactions.

We test this simple hypothesis in SiC and GaAs by comparing our predictions with the measured experimental data of EDs [6], where they exist, and with the LDF method [4,8,9]. We conclude that the 11RIM, which is limited to first and second nearest-neighbour force constant parameters, is adequate for ED predictions. Moreover we believe our comparison of calculations of EDs and phonon frequencies with the other phenomenological models and the measurements suggests common underlying physical concepts. We conclude that it is feasible to predict EDs from phonon properties (rather than just phonon frequencies) and that our technique appears valid when applied to different models. In the light of this work we suggest that the question of phonon property–ED prediction needs to be reappraised.

2. Method

To test the hypothesis stated in the introduction, we begin with the 3RIM. This model derives from the 11RIM when all of the second nearest-neighbour force constants are set to zero. The three parameters of the 3RIM are A and B, the first nearest-neighbour force constant parameters, and Z, the static ionic charge. The parameters A and Z are accurately determined by the measured zone centre phonon frequencies from the first-order Raman scattering data. The parameter B is determined by minimizing the quantity

$$\chi^2 = \sum_{ij=12,44} \left(\frac{C_{ij_{\text{th}}} - C_{ij_{\text{exp}}}}{\sigma_{ij_{\text{exp}}}} \right)^2$$

where $C_{ij_{\text{th,exp}}}$ are the theoretical and measured elastic constants and $\sigma_{ij_{\text{exp}}}$ are the experimental uncertainties. The measured elastic constants for SiC and GaAs are taken from [10] and [11] respectively.

Only one well defined minimum is found and that determines B. These parameters form the limited 3RIM from which we compute the phonon frequencies as well as the EDs at the critical points (CPs) in the zone.

Table 1 compares the predicted EDs of the 3RIM for SiC with the LDF method calculations [9] since measurements are not available. We tabulate the predicted EDs of the 3RIM for GaAs, the four available measurements of GaAs and the LDF method calculations. The predictions of the 3RIM for GaAs are shown to be in good agreement with the measurements for LO(X) and LA(X) but they differ by 33% for LO(L) and 21% for LA(L). The LDF predictions have similar variations. In the case of SiC the 3RIM predictions agree, to within 3%, with the nine EDs calculated by the LDF method [9]. We conclude that the 3RIM is reliable for predictions to within 33% in the zone although this is material dependent. As a next step we take the three parameters of 3RIM as the basis for calculation in the 11RIM. We determine the remaining eight parameters by using the equations of motion at the four CPs at X and L and two CPs at K in the zone. In the spirit of the harmonic approximation we

Table 1. The calculated eigendisplacements $|\omega_C|$, $|\omega_{Ga}|$, at the CPs in SiC and GaAs respectively.

CP	3RIM (SiC)	LDF [9] (SiC)	Measured [6] (GaAs)	3RIM (GaAs)	LDF [4, 8] (GaAs)
LO(Γ)	0.837	—	—	0.720	—
TO(Γ)	0.837	0.837	—	0.720	—
LO(L)	1	1	0.58±0.07	0.769	0.757
LA(L)	0	0.003	0.81±0.05	0.639	0.653
TO(L)	0.853	0.859	—	0.721	0.721
TA(L)	0.521	0.511	—	0.639	0.693
LO(X)	1	1	1	1	1
LA(X)	0	0	0	0	0
TO(X)	0.881	0.889	—	0.723	0.650
TA(X)	0.473	0.458	—	0.693	0.750
$1O\Sigma$(K)	0.913	—	—	0.723	—
$11O\Sigma$(K)	0.994	—	—	0.830	—
$11A\Sigma$(K)	0.071	—	—	0.558	—
TO(K)	0.872	—	—	0.725	—
$1A\Sigma$(K)	0.416	—	—	0.689	—
TA(K)	0.490	—	—	0.691	—

allow the input frequencies to vary by up to 6% from the measured values for SiC but again seek minima with respect to the predicted and measured elastic constants. For GaAs the typical input frequency variation is 8% although variations up to 62% were necessary for the TA modes.

For conciseness we have converted all atomic displacement ratios of two atoms into their equivalent EDs. The ED of an atom (J), $|\omega_J|$, is defined as the product of the atomic displacement times the square root of the mass. The details of the 11RIM and the notation of the parameters has been previously given in [12] but we note that the atom with the lighter mass is placed at the origin of the unit cell, while the atom with heavier mass is placed at $(1,1,1)2a/4$ (where $2a$ is the lattice spacing: for SiC = 4.36 Å and for GaAs = 5.6532 Å).

3. Results

Here we give the results of our calculations for SiC and GaAs separately. Figure 1 gives phonon dispersion curves of SiC as measured by Raman scattering [13–15] and calculated by 11RIM using the force constant parameters of table 2. The second-neighbour short-range force constant parameters E_1 and E_2 have significant effects on the [1,ξ,0] phonon dispersions, on some off-symmetry directions and on four of the quasimodes in the [1,1,0] direction away from the long-wavelength limit. In the absence of experimental data for any of these directions, it is not possible to optimize the parameter values and we have therefore refrained from giving them any values at all and set them to zero. It should be noted that these two parameters have no effect on the dispersions in the [1,0,0] and [1,1,1] directions and they do not contribute to the long-wavelength phonon modes in [1,1,0] direction. In figure 1 the uncertainties in the measured Raman scattering data are not shown, but they were quoted by Feldman *et al* [13–15] to be ±2 cm^{-1} for the zone centre frequencies and ±1% for the rest of the modes in the zone.

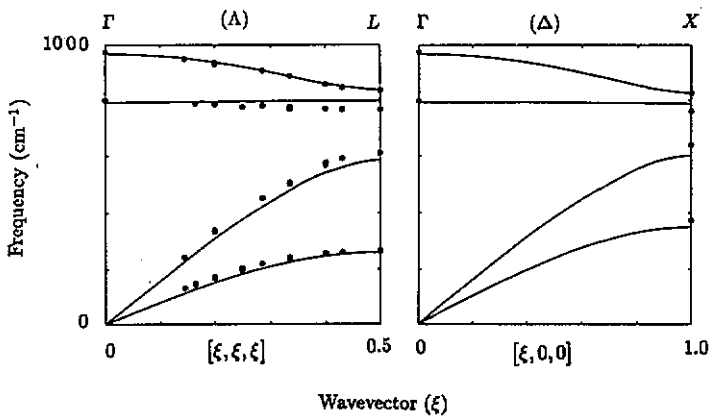

Figure 1. Phonon dispersion curves in SiC calculated using 11RIM. The circles are the experimental points from [13–15].

Table 2. The eleven parameters of the RIM for SiC. The parameters are in units of 10^2 N m^{-1}.

Parameter	11RIM
A	+0.905 68
B	+0.878 19
C_1	+0.045 78
D_1	+0.019 17
E_1	see text
F_1	−0.009 85
C_2	+0.115 85
D_2	+0.060 91
E_2	see text
F_2	−0.063 30
X	+0.243 17

Table 3 gives the calculated CP phonon frequencies of the 11RIM together with the measured Raman scattering data of SiC and the values calculated on the basis of VOSM [9], and the LDF method [9].

Table 4 lists the calculated EDs at the CPs in the zone obtained using the 11RIM, LDF method and VOSM calculations and shows that the EDs of the 11RIM and the LDF method agree to better than 0.005 (i.e. better than 0.5% if EDs are normalized to 1) at all CPs, and 11RIM and VOSM disagree by 0.11 (i.e. effectively 11%) for LA(L), but otherwise agree within 0.017 (i.e. effectively within 1.7%).

Table 5 illustrates the agreement between the measured elastic constants of SiC [10] and the 11RIM calculations to within rounding errors. Note that parameter B for 3RIM was derived by optimizing this fit, but it is clear that introducing the eight extra parameters for 11RIM has not adversely affected this.

Table 6 gives the set of force constant parameters of the 11RIM for GaAs. Table 7 lists the phonon frequencies of GaAs as measured by neutron scattering at room temperature [16] together with those calculated by 11RIM and the LDF method [4, 8]. Note that the LDF calculations included force constants out to third nearest-neighbours and this allowed the better fit to eigenvalues near the zone boundaries.

Table 3. The CP phonon frequencies in cubic SiC. The frequencies are in units of cm^{-1}.

CP	Raman data [13–15]	IIRIM (this work)	LDF [9]	VOSM [9]
LO(Γ)	972	968	—	967
TO(Γ)	796	793	758	794
LO(L)	838	839	845	814
TO(L)	766	798	790	784
LA(L)	610	585	617	617
TA(L)	266,262	260	254	262
LO(X)	829	831	830	830
TO(X)	761	789	755	761
LA(X)	640	602	640	602
TA(X)	373	349	367	383
$1O\Sigma$(K)	—	—	—	825
$1IO\Sigma$(K)	—	—	—	736
$1IA\Sigma$(K)	—	—	—	581
TO(K)	—	768	—	767
$1A\Sigma$(K)	—	—	—	452
TA(K)	—	328	—	355

Table 4. The calculated eigendisplacements $|\omega_C|$, at the CPs in SiC.

CP	IIRIM (this work)	LDF [9]	VOSM [9]
LO(Γ)	0.837	—	0.837
TO(Γ)	0.837	0.837	0.837
LO(L)	1	1	0.994
LA(L)	0	0.003	0.110
TO(L)	0.857	0.859	0.862
TA(L)	0.515	0.511	0.507
LO(X)	1	1	1
LA(X)	0	0	0
TO(X)	0.887	0.889	0.878
TA(X)	0.462	0.458	0.479
$1O\Sigma$(K)	—	—	0.998
$1IO\Sigma$(K)	—	—	0.849
$1IA\Sigma$(K)	—	—	0.098
TO(K)	0.877	—	0.875
$1A\Sigma$(K)	—	—	0.524
TA(K)	0.480	—	0.484

Table 5. The measured and calculated elastic constants for SiC. The parameters are in units of 10^{10} N m^{-2}.

Parameters	Measured [10]	IIRIM (this work)
C_{11}	36.3	36.3
C_{12}	15.4	15.4
C_{44}	14.9	14.9

Table 6. The eleven parameters of the 11RIM for GaAs. The parameters are in units of 10^2 N m^{-1}.

Parameter	11RIM
A	+0.407 33
B	+0.365 00
C_1	+0.032 57
D_1	+0.018 77
E_1	+0.040 00
F_1	−0.012 98
C_2	+0.031 17
D_2	+0.036 45
E_2	−0.035 00
F_2	+0.040 08
X	+0.042 56

Table 8 lists the measured EDs [6] for GaAs, together with the EDs obtained using the parameters listed in table 6 for 11RIM and the EDs deduced by the LDF method [4, 8]. Note that 11RIM agrees with the four available measured values within the quoted experimental uncertainties whereas the LDF calculations for LO(L) and LA(L) are outside the quoted experimental limits.

Table 7. The CP phonon frequencies in GaAs. The frequencies are in units of cm^{-1}.

CP	Measured [16]	11RIM (this work)	LDF [4, 8]
LO(Γ)	285.0±6.7	291	300
TO(Γ)	267.3±2.7	269	273, 286
LO(L)	238.3±2.3	250	241
TO(L)	261.3±4.0	272	279
LA(L)	208.7±3.3	214	203
TA(L)	62.0±0.7	91	65
LO(X)	240.7±5.0	234	252
TO(X)	252.0±3.0	273	265
LA(X)	226.7±2.0	224	240
TA(X)	78.7±0.5	128	62
$1O\Sigma$(K)	264.7±4.0	279	—
$1IO\Sigma$(K)	217.3±4.0	235	—
$1IA\Sigma$(K)	198.7±3.7	207	—
TO(K)	—	273	—
$IA\Sigma$(K)	111.3±2.3	145	—
TA(K)	79.3±1.3	118	—

Table 9 confirms that calculated elastic constants of the 11RIM are in good agreement with the measured values [11] for GaAs.

4. Discussion

It is apparent from figure 1 and table 3 that the calculated dispersion curves of 11RIM describe the measured frequency data of SiC to within 6%. Similar errors at the zone boundaries are evident in the frequency calculations of the LDF method

Table 8. The eigendisplacements $|\omega_{Ga}|$, at the CPs in GaAs.

CP	Measured [6]	11RIM (this work)	LDF [4, 8]
LO(Γ)	—	0.720	—
TO(Γ)	—	0.720	0.720
LO(L)	0.58±0.07	0.615	0.757
LA(L)	0.81±0.05	0.788	0.653
TO(L)	—	0.707	0.721
TA(L)	—	0.707	0.693
LO(X)	1	1	1
LA(X)	0	0	0
TO(X)	—	0.667	0.650
TA(X)	—	0.745	0.750
$1O\Sigma$(K)	—	0.755	—
$1IO\Sigma$(K)	—	0.259	—
$1IA\Sigma$(K)	—	0.953	—
TO(K)	—	0.682	—
$1A\Sigma$(K)	—	0.674	—
TA(K)	—	0.731	—

and the VOSM (table 3). Given that any model or method makes approximations to yield a tractable problem, these frequency variations may be considered reasonable. Variations must be expected to arise both from the anharmonicity of real solids and from the neglect of the short-range part of the forces from further neighbours. These further-neighbour forces make important contributions to the flatness of the TA dispersion curves towards the zone boundaries [17]. It appears in the case of SiC that both the anharmonic forces and the contribution of the short-range forces from further neighbours are quite small. From table 4 it is apparent that 11RIM predicts similar EDs in SiC to both the LDF method and the VOSM calculations. The predictions of 11RIM, the LDF and the VOSM agree to within 1% at most of the CPs. Slightly larger variations occur in the VOSM predictions for the EDs in the LA(L) and TA(X) modes. We also note that the EDs of 11RIM for the LO(L) and LA(L) do indeed tend to unity and zero respectively as expected [9].

Table 9. The measured and calculated elastic constants for GaAs. The parameters are in units of 10^{10} N m^{-2}.

Parameters	Measured [11]	11RIM (this work)
C_{11}	11.84±0.04	11.81
C_{12}	5.37±0.16	5.40
C_{44}	5.91±0.02	5.92

We now consider the predictions of the 11RIM for the CP phonon frequencies in GaAs given in table 7. Comparison of the measured values and those obtained using 11RIM shows agreement to within 8% at most of the CPs. Large variations occur for the TA modes towards the zone boundaries. Similar qualitative differences also arise in the LDF method predictions. The LDF method calculations have shown that forces up to and including fifth-nearest neighbours are required in a model to

reproduce the measured flatness of the TA mode in GaAs. In the approximation that Ga and As atomic masses are identical the crystal structure becomes diamond-like. It is well known that in diamond-like crystals simple Born–von Kármán type models require that the short-range part of the interactions be taken to at least fifth- or sixth-nearest neighbours to reproduce the flatness of the dispersion curves towards the zone boundaries [17].

Table 8 shows that the worst-case 11RIM ED prediction is within 6% of the most-likely measured value and still well within the quoted experimental uncertainty. For those CPs where the measurements have not been made, 11RIM and the LDF predictions agree to within 4%. Table 1 shows that 3RIM and the LDF agree to within 12% at all of the CPs and in general much better. Both 3RIM and the LDF show differences of up to 30% from the measured EDs in LO(L) and LA(L). This divergence is not apparent in the 11RIM. This suggests that 3RIM itself has reasonable predictive powers but that 11RIM is better.

To what extent do the force constants of 11RIM represent real physical parameters of the solids? The dominant contribution to the EDs of 11RIM arise from the first-neighbour constants which are determined by 3RIM. If these parameters have genuine physical significance we might expect a similar approach to yield similar results in other models. Table 10 lists the calculated EDs in GaAs obtained using 3RIM, and three different shell models in which only the first-nearest neighbours are taken into account (1SM refers to the c(i) model of [16]; 1DDM is from [18]; and 1OVSM refers to OSM3 of [6]). We have not sought to optimize these other models with respect to long-wavelength properties but have merely recalculated the EDs when all but the (published) first nearest-neighbour parameters are set to zero. Table 10 demonstrates that in general the first-order EDs of all these limited models converge to better than 9%. The only significant variation is for the ED of the LA(L) mode of the 1OVSM. This convergence of the ED predictions suggests that the limited models have underlying physical similarity and by inference the full models have the same inherent similarity. As Leigh *et al* have noted, the prediction of the force constant parameters of a solid is possible if EDs are taken into account.

Table 10. The calculated eigendisplacements $|\omega_{Ga}|$, at the CPs in GaAs using 3RIM, 1SM, 1OVSM and 1DDM.

CP	3RIM (this work)	1SM [16]	1OVSM [16]	1DDM [18]	Standard deviation
LO(Γ)	0.720	0.720	0.720	0.720	—
TO(Γ)	0.720	0.720	0.720	0.720	—
LO(L)	0.769	0.852	0.921	0.744	7%
LA(L)	0.639	0.523	0.388	0.668	11%
TO(L)	0.721	0.653	0.750	0.731	4%
TA(L)	0.639	0.758	0.662	0.683	5%
LO(X)	1	1	1	1	—
LA(X)	0	0	0	0	—
TO(X)	0.723	0.673	0.791	0.752	4%
TA(X)	0.693	0.740	0.612	0.659	5%

This version of the RIM has genuine predictive ability for EDs. The first-order predictions of 3RIM are accurate to within 6% for SiC and 33% for GaAs. We note that this model utilizes a very limited number of parameters and forms the basis of

11RIM—indeed the crucial nearest neighbour force constants are identical in the two models. At long wavelengths these harmonic models provide a realistic description of the interatomic interactions. The predictions EDs from 3RIM and 11RIM are sufficiently similar to conclude that they are converged and indeed we find that varying the model parameters near the optimized set, leads to a converged ED set. We conclude that the procedure produces a unique parameter set and hence a unique prediction for the EDs.

5. Conclusions

We have established a procedure for the optimization of the force constant parameters of the 11RIM which permits predictions of the EDs. This procedure is based on the assumption that the dominant contribution to the EDs in a harmonic solid comes from the first nearest neighbour forces. The necessary model parameters can then be determined in the long wavelength limit using two zone centre frequencies and the measured elastic constants.

Precise agreement is not expected with the measured phonon frequencies throughout the zone and neither are many parameters necessary to arrive at a first-order prediction of the EDs. The predictions of EDs appear to be improved when second neighbours are included although we still find some differences with measured frequencies.

In GaAs the predicted EDs of 11RIM are well within the experimental uncertainty. In SiC the predicted EDs agree with those of the LDF method to better than 1% for all the CPs. We concluded that, when correctly optimized, the 11RIM ED predictions should always be reliable to within 10% overall, possibly within 1%, and certainly as good as any other currently available mathematical model.

The convergence of the calculations for the EDs of the 11RIM, the LDF method and the VOSM strongly suggests underlying physical similarity. The convergence of the limited 3RIM with a number of first neighbour models gives weight to this conclusion. If such different models are capable of generating essentially identical results a stronger conlusion might be suggested. *Given proper optimization,* all physically reasonable models lead to a converging set of EDs and hence realistic estimates of force constant parameters. This convergence may be confirmed by comparison if the EDs with measurements or the LDF predictions. Other aspects of this work, such as our clear demonstration that published sets of eigenvalues and eigenvectors are *not* model specific, will be dealt with elsewhere.

Acknowledgments

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