Lattice dynamics for fcc rare gas solids Ne, Ar, and Kr from *ab initio* potentials

Gloria E. Moyano and Peter Schwerdtfeger[*]

*Centre of Theoretical Chemistry and Physics, Institute of Fundamental Sciences, Massey University (Albany Campus),
Private Bag 102904, North Shore MSC, Auckland, New Zealand*

Krzysztof Rosciszewski[†]

Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany

Specific heat at constant volume calculations are presented from lattice dynamic calculations of harmonic phonon branches for the face-centered cubic crystals of Ne, Ar, and Kr using *ab initio* two-body potentials. The calculated temperature-dependent specific heats and derived Debye temperatures are in good agreement with experimental results. The unusually low Debye temperature of Ne in comparison to the heavier rare gas solids is analyzed in detail.

I. INTRODUCTION

Crystal lattice dynamics theory has evolved from the need to accurately predict properties such as the phonon spectra and thermodynamic quantities of solids. The rare gas solids (RGS's) have constituted a special case, as modeling these systems does not require consideration of strong bonding interactions, many-neighbor interactions, or free electron gas.[1] The solids of the heavier rare gases, for which quantum effects can be neglected, are treated on a common basis. The appropriateness of a particular approach can be assessed by comparison with experimental phonon dispersion curves, temperature dependences of the specific heat $C_v(T)$, and other measurable quantities.

Recent empirical calculations of the phonon spectra of some fcc lattices,[2] from measured elastic constants, provided an argument in favor of the assumption that nearest-neighbor interactions are sufficient to accurately model the lattices of Xe, Kr, Ar, and even Ne. The agreement between the calculated and the experimental temperature dependences of the specific heat at constant volume served in such study as a criterion to evaluate the calculated phonon densities. We recall that the Cauchy equality $C_{12}=C_{44}$, where C_{12} and C_{44} represent two of the three distinguishable elastic constants of a cubic solid, holds reasonably well for the RGS's of the elements mentioned above, at temperatures between 5 and 25 K,[3–5] and towards the zero-pressure limit (see predictions compared with experimental data in Ref. 6). The fulfillment of Cauchy's equality is used as an indicator of the suitability of pair additive potentials to model the solids.[7] The findings cited from empirical calculations are consistent with a history of theoretical approaches: namely, models of the RGS lattice dynamics based on sums of pair potentials, often of the Lennard-Jones (LJ) type,[8] to represent the potential of the solid.[1,6,9–12] Thus theoretical studies of the RGS's have focused on the development of realistic pair potentials, as well as on the evaluation of corrections by many-body interactions, multiple neighbors, and anharmonic effects.

The homology of the RGS's has also been investigated from the analysis of their phonon spectra as well as from the study of their thermodynamics variables.[1,13] Such homology,

which holds in the case of argon, krypton, and xenon, justifies the use of a common model for the solid state of these systems. Quantum effects become important for solid Ne and are necessary to describe solid He. The thermodynamic properties of the RGS's have thus been calculated by Monte Carlo and molecular dynamics simulations using LJ potentials as well as other sophisticated pair potentials, often parametrized empirically.[12,14–18] For example, specific heats at constant volume for argon, determined by Monte Carlo and molecular dynamics calculations, showed reasonable agreement with experimental data at temperatures in the range 20–90 K.[14,15] Those calculations were based on models of the fcc lattice with only 108 particles, using the Wigner-Kirkwood expansion of the free energy. Such predictions of the specific heat reported in the literature show discrepancies which are sensitive upon the methodologies used.[1,14,15] However, for a given method there seems to be less sensitivity to the choice of two-body potentials. This case is illustrated by the specific heats of argon calculated by Asger and Usnami,[14] where no significant differences could be found by using either LJ or Aziz[19] potentials. However, the responses to the effects here considered have been found to be variable depending upon the property.

Anharmonic effects tend to be important for quantities like phonons and specific heats of RGS's at higher temperatures[2,11,18] and pressures,[6] and when considering quantum solids like Ne or He. On the other hand, many body effects of third or higher orders are more difficult to investigate due to the computational cost and the challenges to obtain an accurate description of these interactions.[6,15,20] However, where attempts to evaluate the contributions of three-body forces have been made, these forces have turned out to be negligible at low pressures, particularly in calculations of the specific heat.[15]

In a previous work we used *ab initio* many-body interaction expansions to study the RGS crystal lattices.[6] We found that the many-body expansion converges rapidly at distances higher than the hard-sphere radius, so that we can accurately predict lattice parameters and cohesive energies using only two-body terms. These two-body potentials were constructed by fitting pointwise *ab initio* calculations for the diatomics of Kr, Ar, Ne, and He to an extension of the LJ formula. In this

paper the RGS lattice dynamics is further studied using the extended LJ *ab initio* pair potentials mentioned above for Ne, Ar, and Kr. We calculate the harmonic phonon spectra by diagonalization of the dynamic matrix for an fcc cluster in reciprocal space and then use these phonon frequencies to obtain the specific heat of the lattices. This constitutes a complete first-principles calculation of the lattice dynamics for the RGS's. We compare the results with analogous ones obtained using other empirical potentials as well as with available experimental data.

II. METHOD

The potential energy for the lattices is expressed as a sum of two-body interatomic potentials $V^{(2)}(r)$ as described in our previous paper,[6] which were obtained from accurate *ab initio* energies for the systems He_2,[21] Ne_2,[22] Ar_2,[21] and Kr_2.[23] The data points for those potential curves were fitted to an extended LJ-type (ELJ-type) potential

$$V^{(2)}(r_{ij}) = \sum_{k=1}^{n} c_{2k+4} r_{ij}^{-2k-4} \qquad (1)$$

by a linear-least squares procedure. r_{ij} is the internuclear distance between atoms i and j. The fitting parameters c_{2k+4} are given in Ref. [6]. Phonon frequencies and branches along certain directions of space were calculated, within the harmonic approximation, for fcc clusters of 8589 atoms for Ne, Ar, and Kr. It was shown previously that for such cluster sizes the phonon branches are converged out to high accuracy.[20] The dynamic matrices were constructed and diagonalized in reciprocal space, using a grid of k points homogeneous in the Brillouin zone. To calculate the phonon branches we implemented the two-body potentials in the code developed by Rosciszewski *et al.*,[20] and then interfaced it with the solid-state code SAMBA.[24] The latter sorts the phonon frequencies to produce a frequency distribution $g(\omega)$ used to calculate the temperature dependences of the specific heat at zero pressure. The specific heat at constant volume was thus evaluated by summing over all phonon frequencies according to the well-known expression

$$C_v(T) = \frac{R}{N} \sum_{i=1}^{3N} \left(\frac{\hbar \omega_i}{k_B T} \right)^2 \frac{e^{\hbar \omega_i / k_B T}}{(e^{\hbar \omega_i / k_B T} - 1)^2}$$

$$= 3R \int_0^{\omega_{max}} d\omega \, g(\omega) \left[\frac{\hbar \omega / 2 k_B T}{\sinh(\hbar \omega / 2 k_B T)} \right]^2, \qquad (2)$$

where N is the number of atoms which yields $3N$ phonon frequencies ω_i, T the temperature, k_B the Boltzmann constant, and $N_A k_B = R$ with N_A being Avogadro's number. The calculations are also performed using the empirical two-body potentials of LJ (Ref. [25]) and HFD-B (derived from repulsive Hartree-Fock plus dispersion using low temperature second virial data, see Refs. [19] and [26–28]) for comparison.

III. RESULTS AND DISCUSSION

Figure 1 shows the phonon dispersion curves for neon, argon, and krypton. Most of the previous calculations of
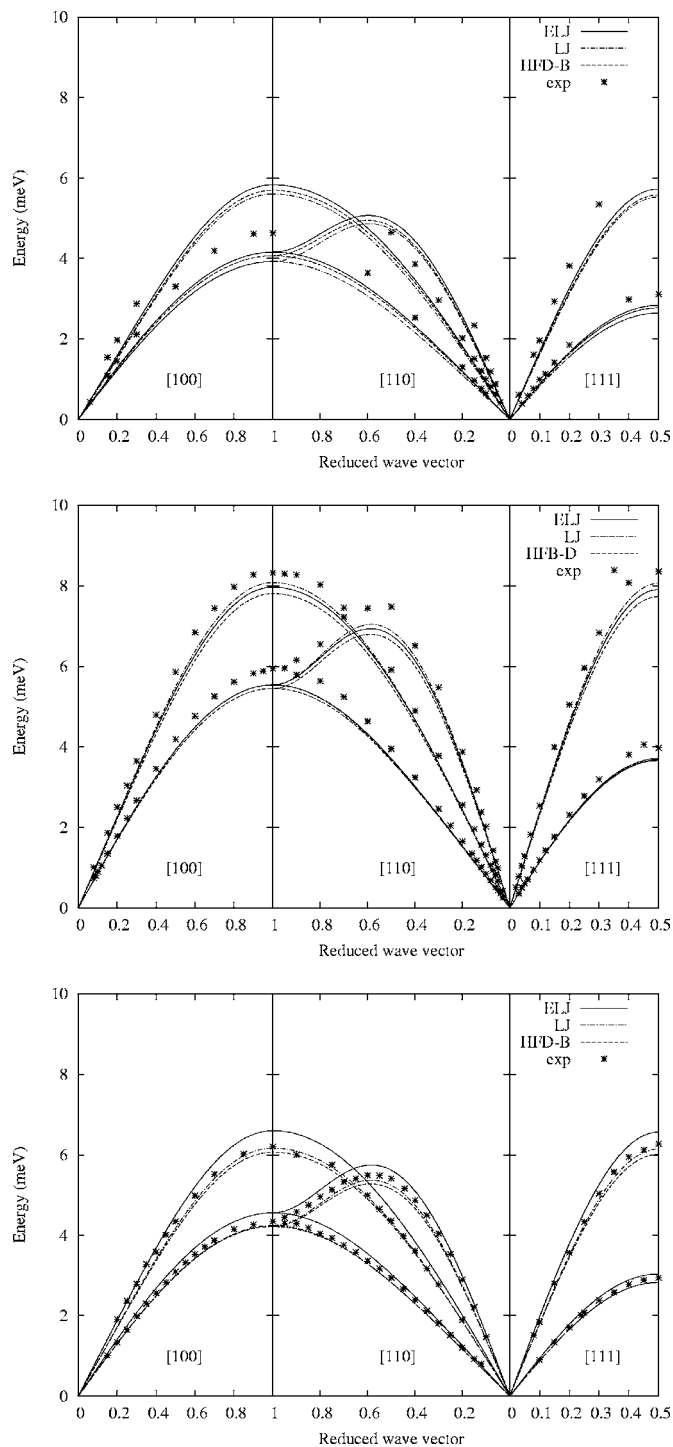

FIG. 1. From the top to the bottom: phonon dispersion of neon, argon, and krypton obtained from two-body potentials (see text). Experimental data from Refs. [3–5] are represented with a star point type.

phonon dispersion curves have been performed for solid argon, using potentials parametrized empirically. Unlike in this paper, the main pursuit of these studies had been the temperature dependences of the phonons, particularly near melting.[1,9,11] However, they have also produced phonon frequencies in agreement with the observed values near 0 K. The quasiharmonic and the self-consistent harmonic approxi-

mations, with several corrections, have been used along with empirical pair potentials like the LJ, the Bobetic-Barker,[12] the Azis-Chen, and variants such as the HFD-B developed by Aziz and co-workers.[19,26–28] The contribution of three-body forces has also been considered through Axilrod-Teller-Muto terms.[9]

Figure 1 shows that the three types of two-body potentials chosen (LJ, HFD-B, and *ab initio* ELJ) predict phonon branches with slight discrepancies between them, which are at most of 8% in the case of Kr and 4% in the cases of argon and neon. When comparing the predicted and the experimentally measured phonons, the *ab initio* ELJ potential gives the closest results for neon and the most deviated for krypton. This is expected as very accurate *ab initio* potential curves are available for the light elements like helium or neon. To include electron correlation and relativistic effects (including spin-orbit interactions) becomes increasingly more difficult for the heavier rare gases, resulting in larger discrepancies in the *ab initio* Kr_2 potential by Tao.[23] The largest differences between the phonon frequencies produced by the ELJ potential and the experimental values amount to 14% in the case of neon and 9% in the cases of argon and krypton. As a reference, the largest experimental uncertainties in the phonon energies are 7.1% in the case of neon at 6.5 K,[5] 3.2% for argon at 10 K,[4] and 6.3% for krypton at 10 K.[3]

Taking the predicted phonon frequencies as a criterion, the *ab initio* potentials perform as good as the pair potentials parametrized empirically, except for Kr. The model used here underestimates the phonon frequencies, and a more precise treatment requires the inclusion of three-body forces (especially for the heavier rare gases) and anharmonicity effects (especially for the lighter rare gases). Also, the largest discrepancies between the predictions based on the various types of two bodies occur for the longitudinal branches at high values of the reduced wave number q. As pointed out by Glyde and Smoes,[9] the LJ potential performed very well in the prediction of the phonons close to 0 K, and some pair potentials turned out to be indistinguishable with regard to the predicted phonon frequencies at low temperature. However, clear differences appeared when considering higher temperatures and temperature dependences. The same authors also concluded that the longitudinal branches are more sensitive to variations in the methodology and particularly to the inclusion of three-body forces.[9]

Figure 2 shows the temperature dependence of the constant-volume specific heat for neon, argon, and krypton. The experimental values at low T are based on the phonon densities calculated from the spectra and extrapolated to 0 K. These specific heats are compared with the experimental data available for the RGS's between 0 K and temperatures close to the melting point. Once again, the choice of pair potential does not represent significant variations, although the $C_v(T)$ curve predicted for krypton with the ELJ potential clearly diverges from the calculated with the empirical LJ and the HFD-B potentials for the reasons mentioned above. The $C_v(T)$ curve corresponding to the ELJ potential is always below those of the empirical potentials, and the largest differences between the predicted curves are approximately 11% around 10 K. The predicted $C_v(T)$ curves for argon are all very similar, with discrepancies of 2% or less in the range

of temperatures considered, which are mostly associated with the HFD-B potential.

Comparison of the predicted $C_v(T)$ curves with the smoothed experimental data for solid argon and krypton determined by Finegold and Phillips[33] reveals excellent agreement for argon and small discrepancies (of less than 1 J mol^{-1} K^{-1}) for krypton. Interestingly, the closest agreement with the experimental curve for krypton is obtained using the ELJ potential, which might be due to error compensation. The $C_v(T)$ curves predicted here for neon differ from the experimental ones[29,30] more than for the other RGS's. The predicted specific heats for neon overestimate the experimental values over the range of temperatures considered by (2 J mol^{-1} K^{-1} or less), and the best prediction is obtained using the ELJ potential. It is important to note that the experimental uncertainties amount to ±1.6 J mol^{-1} K^{-1}) in the specific heats of neon reported by Batchelder *et al.*,[29] and 2% in the smoothed values by Fenichel and Serin.[30] The larger discrepancies from experiment found here for the specific heats of neon in comparison with argon and krypton are expected considering the increasing importance of anharmonic effects in the solid state of the lighter rare gases which we have not taken into account.

Other predictions of the specific heat already reported resorted heavily to empirical pair potentials and proceeded through the calculation of the free energy of the solid. Several approximations based on the self-consistent phonon theories were tried, mainly for argon, with a focus on ranges of higher temperatures. However, even in this scenario where the theories were expected to perform best, reasonable agreement with experiment was difficult to achieve (see Ref. 31 and references cited therein). Computer simulation techniques such as Monte Carlo and molecular dynamics have also been applied in order to calculate the temperature dependences of the specific heat for argon, concentrating as well on higher-temperature ranges,[1,14–16] attaining reasonably good agreement with experimental curves. As relevant to the discussion of our work Asger and Usnami[14] found very similar the performances of the LJ and sophisticated empirical pair potentials in the prediction of the $C_v(T)$ curves of argon, while some discrepancies between analogous predictions for the case of neon. They also observed more discrepancy between the predicted and the experimental curves for neon than for argon. However, our specific heat curves are the closest to experiment in the low-temperature region reported so far.

Finally we compare the $C_v(T)$ curves for argon for the three different approximations in Fig. 3, the Einstein approximation where only one atom is moved in the field of all other atoms [$N=1$ in Eq. (2)], the Debye approximation

$$C_v^{Debye}(T) = 9R\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2}, \qquad (3)$$

where θ_D is the Debye temperature, and our more concise treatment including all phonon frequencies and using the ELJ potential. The calculated Einstein frequency of 50.7 cm^{-1} from Ref. 6 and the experimentally derived Debye temperature of $\theta_D = 91.8$ K from Refs. 1 and 2 is taken.
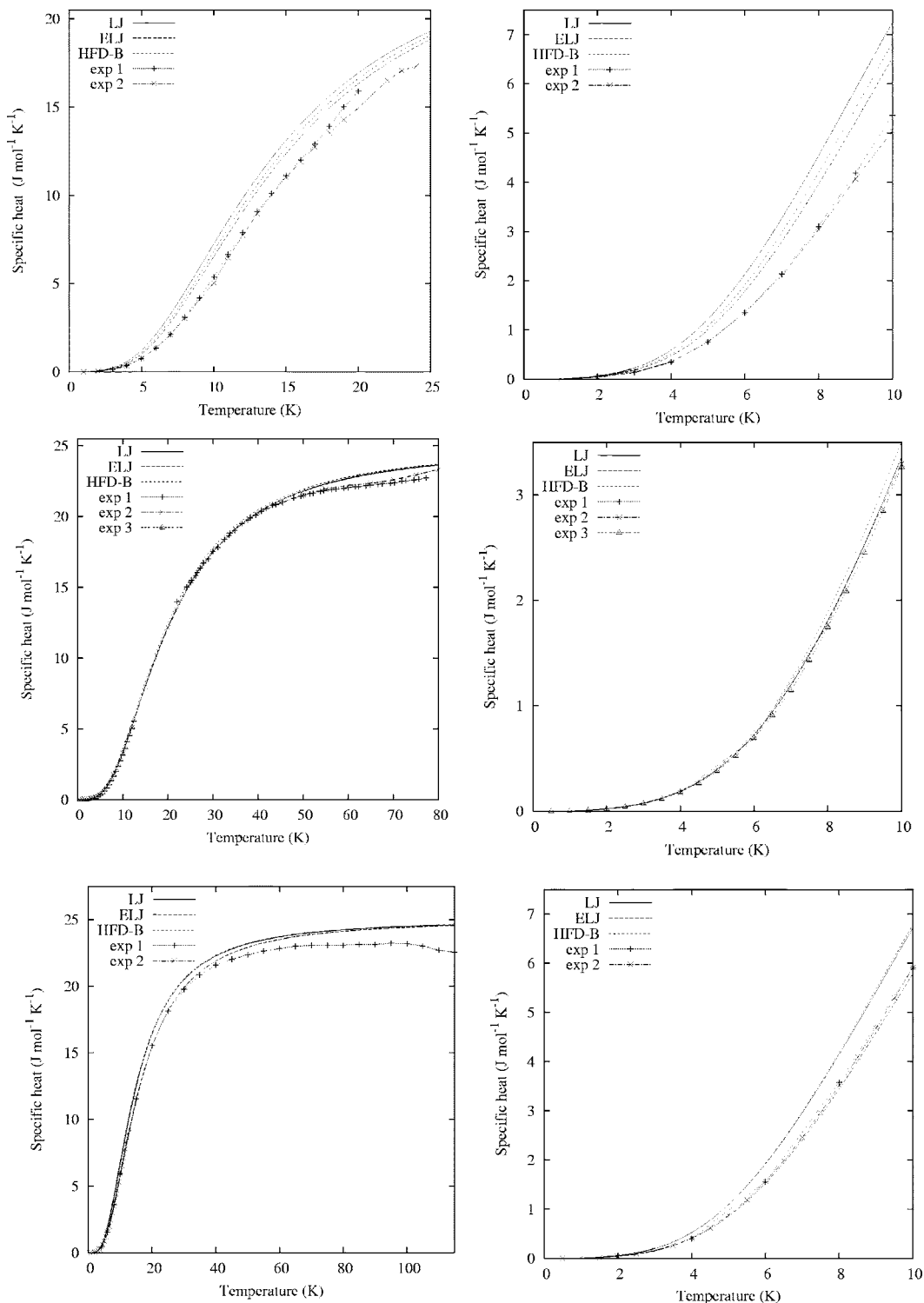
FIG. 2. From the top to the bottom: specific heat of neon, argon, and krypton. From the left to the right: high- and low-temperature region of the specific heat. Experimental data: for neon, exp 1 from Ref. 29 and exp 2 from Ref. 30; for argon, exp 1 from Ref. 31, exp 2 from Ref. 32, and exp 3 from Ref. 33; for krypton, exp 1 from Ref. 34 and exp 2 from Ref. 33.

Figure 3 shows that neither the Einstein nor the Debye approximation works particularly well for the whole temperature range.

The low-temperature behavior in Fig. 2 shows an interesting anomaly. If we take the well-known low-temperature approximation

$$C_v(T) = aT^3 \quad \text{with } a = \frac{12\pi^4 R}{5\theta_D^3},\tag{4}$$

we obtain for the constant a from our calculations using the ELJ potential (in J mol^{-1} K^{-4}) 6.04×10^{-3} for Ne,
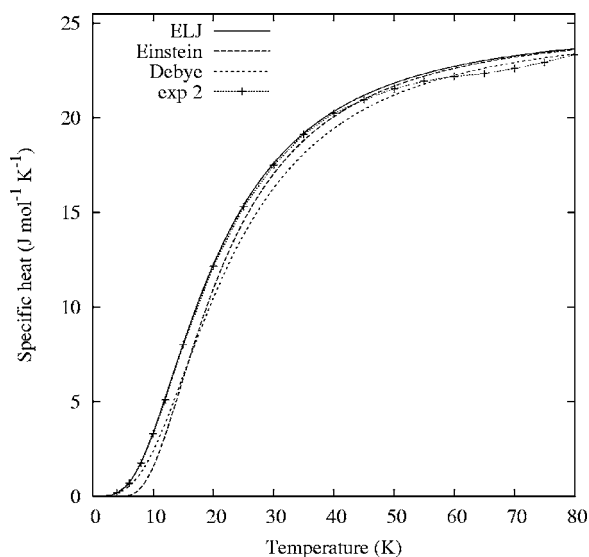
FIG. 3. Specific heat of argon in three different approximations (see text). Experimental values exp 2 from.[32]

FIG. 4. Debye temperature versus the diatomic harmonic vibrational frequencies from Ne to Xe (see text for details).

2.59×10^{-3} for Ar, and 5.28×10^{-3} for Kr. From the experimental data (see Fig. 2) we obtain 4.02×10^{-3} for Ne, 2.52×10^{-3} for Ar, and 5.32×10^{-3} for Kr. Except for Ne we are in good agreement with experiment. According to Eq. (4) this distinct anomaly in the trend down the group of rare gases is also reflected in the Debye temperature. From our calculations we get 68.5 K for Ne, 90.8 K for Ar, and 71.6 K for Kr. This compares well with experiment where we have 75.1 K for Ne, 91.8 K for Ar, and 72.5 K for Kr in the low-temperature limit.[1,2] Hence, the data do not show a monotonic decrease in the Debye temperature if we go down the group of rare gases in the periodic table as we expect from the increasing mass. We try to explain this anomaly using the LJ ansatz,[8] which is known to work reasonably well for the rare gases.[36]

From a LJ potential

$$V(r) = -c_6 r^{-6} + c_{12} r^{-12}, \qquad (5)$$

where $c_6, c_{12} > 0$ we obtain for the potential of a Bravais lattice (see Ref. 6)

$$V_s(R) = -L_6 c_6 R^{-6} + L_{12} c_{12} R^{-12}, \qquad (6)$$

where the L_n coefficients are the Lennard-Jones-Ingham parameters.[35] r is the distance in the diatomic rare gas and R the nearest-neighbor distance in the solid (fcc in our case). We define the dissociation energy D_e, cohesive energy E_{coh}, force constant of the diatomic rare gas k_e, and symmetric solid-state force constant f_e^s as

$$D_e = -V(r_e), \quad E_{coh} = -V_s(R_e), \quad k_e = \left. \frac{\partial^2 V(r)}{\partial^2 r} \right|_{r_e}, \quad (7)$$
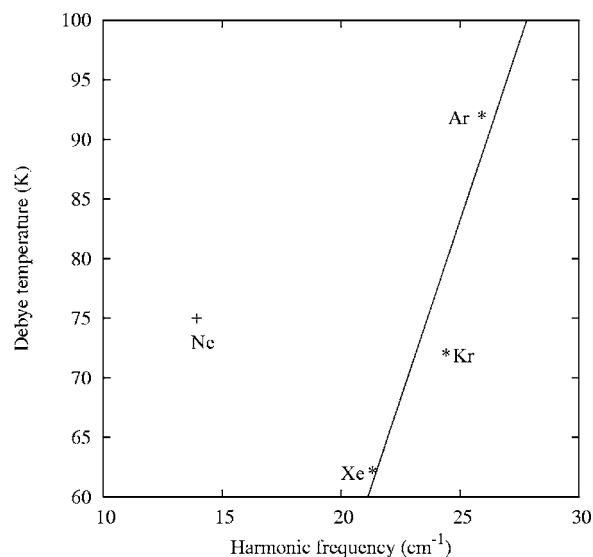
$$f_e^s = \left. \frac{\partial^2 V_s(R)}{\partial^2 R} \right|_{R_e},$$

where r_e and R_e are the equilibrium distances of the diatomic and solid, respectively. After some algebraic manipulations we obtain

$$f_e^s = \frac{1}{2} L_6^{7/3} L_{12}^{-4/3} k_e. \qquad (8)$$

We now argue the following way. f_e^s is the force it takes to expand symmetrically the solid—that is, changing all nearest-neighbor distances to $R_e + \delta R$. In a molecule this relates to the symmetric stretching mode and is characterized by largest frequency of the coupled stretching modes. Similarly we argue that f_e^s is related to the maximum phonon frequency; that is, we have $\omega_{max} = \sqrt{f_e^s / \mu}$ where μ is the reduced mass of this mode. Furthermore, from previous studies we know that $\omega_{max} \approx 3\omega_E/2$, where ω_E is the Einstein frequency. Using the Lennard-Jones-Ingham parameters for the fcc lattice in Ref. 6 we get $\omega_E \approx 2\omega_e$. As the Debye frequency $\omega_D \sim \omega_E$ and $k_B \theta_D = \hbar \omega_D$ we get $\theta_D \sim \omega_e$. Indeed, the vibrational harmonic frequencies for the dimers show the same anomaly; i.e., ω_e is 13.7 cm^{-1} for Ne$_2$, 25.7 cm^{-1} for Ar$_2$, 24.2 cm^{-1} for Kr$_2$, 21.1 cm^{-1} for Xe$_2$, and 17.3 cm^{-1} for Rn$_2$.[37] Here we take Xe and Rn for comparison, the latter taken from relativistic coupled cluster calculations by Runeberg and Pyykkö.[38] Converting these into force constants k_e we get (in N m^{-1}) 0.11 for Ne$_2$, 0.78 for Ar$_2$, 1.45 for Kr$_2$, 1.71 for Xe$_2$, and 1.96 for Rn$_2$. Hence the force constants increase monotonically with increasing atomic number, as are the reduced masses. It is therefore the rather small force constant for the Ne-Ne interaction which causes this anomaly. From argon onwards the trend is dominated by the increasing mass of the rare gase atoms.

This effect seems to propagate into the solid state as it is also observed in the corresponding Debye temperatures.

Figure 4 shows a plot of the experimentally determined Debye temperatures from the solid state[1,2] against the harmonic vibrational frequencies of the rare gas dimers.[37] It clearly shows that Ne is not following the linear regression found for the heavier rare gases. This is due to the strong anharmonicity effects in both solid Ne and Ne_2. Furthermore, many-body effects in the interaction potential become more important in the heavier rare gas systems. We note that a much smoother trend is found between the dissociation energies D_e of the rare gas diatomics and the cohesive energies E_{coh} of the solids.[38] Extrapolating to the $\omega_e = 17.3$ cm^{-1} for Rn we obtain a Debye temperature of 36 K for solid Rn. This is much lower compared to the 90 K value empirically predicted by Kazragis, Surotkevicius, and Liksiene.[39]

IV. CONCLUDING REMARKS

Results from lattice dynamic calculations which produced the phonon branches for fcc Ne, Ar, and Kr showed good agreement for constant-volume specific heat calculations with experimental data. Further work on the evaluation of many-body effects, anharmonic corrections, and more precise potentials for the heavier rare gases is required to produce more accurate results, which is part of our future investigation. The calculations of three-body effects will be expensive in computer time, and we expect the results to cause only minor changes at low pressures, in agreement with our previous study.[6] We established a useful relationship between the harmonic vibrational frequency of the rare gas dimer and the Einstein frequency of the solid, which may be used only if three- or higher-body forces and anharmonicity effects are negligible.

ACKNOWLEDGMENT

*Electronic address: p.a.schwerdtfeger@massey.ac.nz

†Also at the Institute of Physics, Jagellonian University, Reymonta 4, Pl 30-059 Krakow, Poland.

[1] M. L. Klein and J. A. Venables, *Rare Gas Solids* (Academic Press, London, 1976), Vol. 1.

[2] S. O. Feodosyev, I. A. Gospodarev, V. O. Kruglov, and E. V. Manzhelii, J. Low Temp. Phys. **139**, 651 (2005).

[3] J. Skalyo, Y. Endoh, and G. Shirane, Phys. Rev. B **9**, 1797 (1974).

[4] Y. Fujii, N. A. Lurie, R. Pynn, and G. Shirane, Phys. Rev. B **10**, 3647 (1974).

[5] Y. Endoh, G. Shirane, and J. Skalyo, Phys. Rev. B **11**, 1681 (1975).

[6] P. Schwerdtfeger, N. Gaston, R. P. Krawczyk, R. Tonner, and G. E. Moyano, Phys. Rev. B **73**, 064112 (2006).

[7] H. Cox, R. L. Johnston, and J. Murrell, J. Solid State Chem. **145**, 517 (1999).

[8] J. E. Jones, Proc. R. Soc. London, Ser. A **106**, 709 (1924).

[9] H. R. Glyde and M. G. Smoes, Phys. Rev. B **22**, 6391 (1980).

[10] A. I. Karasevskii and W. B. Holzapfel, Phys. Rev. B **67**, 224301 (2003).

[11] E. R. Cowley and G. K. Horton, Phys. Rev. Lett. **58**, 789 (1987).

[12] M. V. Bobetic and J. A. Barker, Phys. Rev. B **28**, 7317 (1983).

[13] V. Ramamurthy and S. B. Rajendraprasad, J. Chem. Phys. **83**, 3590 (1985).

[14] M. Asger and Q. N. Usmani, Physica B **271**, 104 (1999).

[15] J. A. Barker and M. L. Klein, Phys. Rev. B **7**, 4707 (1973).

[16] M. L. Klein, T. R. Koehler, and R. L. Gray, Phys. Rev. B **7**, 1571 (1973).

[17] N. S. Gillis, N. R. Werhamer, and T. R. Koehler, Phys. Rev. **165**, 951 (1968).

[18] R. Ramirez and C. P. Herrero, Phys. Rev. B **72**, 024303 (2005).

[19] R. A. Aziz and M. J. Slaman, Chem. Phys. **130**, 187 (1989).

[20] K. Rosciszewski, B. Paulus, P. Fulde, and H. Stoll, Phys. Rev. B **62**, 5482 (2000).

[21] S. M. Cybulski and R. R. Toczylowski, J. Chem. Phys. **111**, 10520 (1999).

[22] R. Specchio, A. Famulari, and M. Raimondi, J. Mol. Struct.: THEOCHEM **549**, 77 (2001).

[23] F. M. Tao, J. Chem. Phys. **111**, 2407 (1999).

[24] P. Schwerdtfeger, computer code SAMBA, Massey University, Auckland, 2006.

[25] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *The Molecular Theory of Gases and Liquids* (Wiley, New York, 1964).

[26] R. A. Aziz and M. J. Slaman, J. Chem. Phys. **92**, 1030 (1990).

[27] A. K. Dham, A. R. Allmat, W. J. Meath, and R. A. Aziz, Mol. Phys. **67**, 1291 (1989).

[28] A. K. Dham, W. J. Meath, A. R. Allmat, and R. A. Aziz, Chem. Phys. **142**, 173 (1990).

[29] D. N. Batchelder, D. L. Losee, and R. O. Simmons, Phys. Rev. **162**, 767 (1967).

[30] H. Fenichel and B. Serin, Phys. Rev. **142**, 490 (1966).

[31] F. Haenssler, K. Gamper, and B. Serin, J. Low Temp. Phys. **3**, 23 (1970).

[32] O. G. Peterson, D. N. Batchelder, and R. O. Simmons, Phys. Rev. **150**, 703 (1966).

[33] L. Finegold and N. E. Phillips, Phys. Rev. **177**, 1383 (1969).

[34] D. L. Losee and R. O. Simmons, Phys. Rev. **172**, 944 (1968).

[35] J. E. Lennard-Jones and A. E. Ingham, Proc. R. Soc. London, Ser. A **107**, 636 (1925).

[36] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Thomson Learning, Toronto, 1976).

[37] K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure* (Van Nostrand, New York, 1979), Vol. VI.

[38] N. Runeberg and P. Pyykkö, Int. J. Quantum Chem. **66**, 131 (1998).

[39] A. Kazragis, E. F. Surotkevicius, and R. Liksiene, Sb. Tr. Vses. Nauch.-Issled. Inst. Teplorzol. Akust. Stroit. Mater. Izdelii 183 (1972).