Determination of indium melting curve at high pressure by picosecond acoustics
Additional Information

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CONTENTS

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I. INTRODUCTION

This document provides additional details on the determination of pressure and temperature done in the paper of S. Ayrinhac *et al*, "Determination of indium melting curve at high pressure by picosecond acoustics", *Physical Review Materials*, **6**(6), 063403, 2022 [1].

II. SET-UP DETAILS

Ruby[1] and SmSTB[2] were used as pressure-temperature optical calibrants. They were excited by a 488 nm laser source[3], with an output power of approximatively 40 mW. All spectra were recorded with a HR4000 spectrometer[4].

III. METHOD

Whether for Ruby or SmSTB, the wavelength of the considered line depends on T and p :

$$\lambda(p,T) = \lambda_{ref} + \Delta\lambda(\Delta T) + \Delta\lambda(p),$$

where $\lambda_{ref} = \lambda_{p_0,T_0}$, $\Delta T = T - T_0$, and $T_0 = 296$ K=22.85 ^{o}C.

The equations which rely $\Delta\lambda$ in p and T are detailed in the Section I of Supplementary Information of Ref. [1] , and shown in Fig. S1 and Fig. S2, respectively.

However, in the case of ruby, $\Delta\lambda(\Delta T)$ is determined by two models : the Datchi model (see Sec. III A below) and the McCumber model (see Sec. III B).

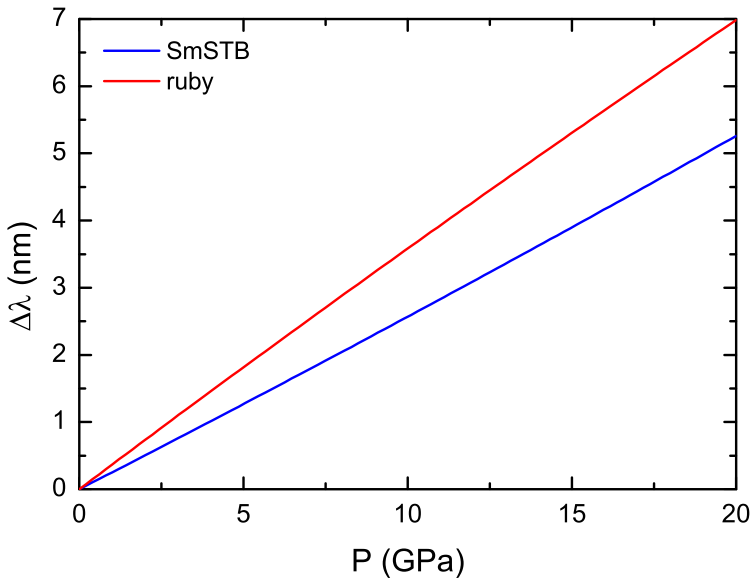
A. The Datchi model

Spectra are smoothed and the position of the maximum is determined (see Fig. S3). The dependance of wavelength λ_{max} with T is given by Eq.(2) in Ref. [2], in the range 296 $K < T <$ 900 K.

B. The McCumber model

The fluorescence signal from the Ruby collected by the HR4000 spectrometer (with a scale expressed in cm^{-1}) is fitted by a sum of 2 Voigt profiles. The Voigt profile is the convolution

[1] Chromium-doped corundum (α-Al_2O_3:Cr^{3+}) with 3000 ppm Cr concentration.
[2] Samarium-doped strontium tetraborate (SrB_4O_7:Sm^{2+}).
[3] Model : Sapphire SF 488-50 CDRH, from Coherent company.
[4] Model HR4C4652, from OceanOptics.



Supplementary Figure S1. Dependance of the wavelength shift $\Delta\lambda$ as a function of p, for two pressure calibrants : SmSTB (blue line) and ruby (red line).

between a lorentzian (width σ) and a gaussian (width Γ) functions. The lorentzian width is fixed by the instrumental line shape at $\sigma = 0.6369914$ cm^{-1}. During the fitting procedure, 6 parameters are free : ν_{R_1}, I_{R_1}, Γ_{R_1}, ν_{R_2}, I_{R_2}, Γ_{R_2} and the background is assumed to be linear with 2 free parameters (slope and intercept), finally a total of 8 parameters are free.

The position of the R_1-line (in cm^{-1}) is related to temperature (according to Eq.(11-12) in Ref. [3]) by the relation

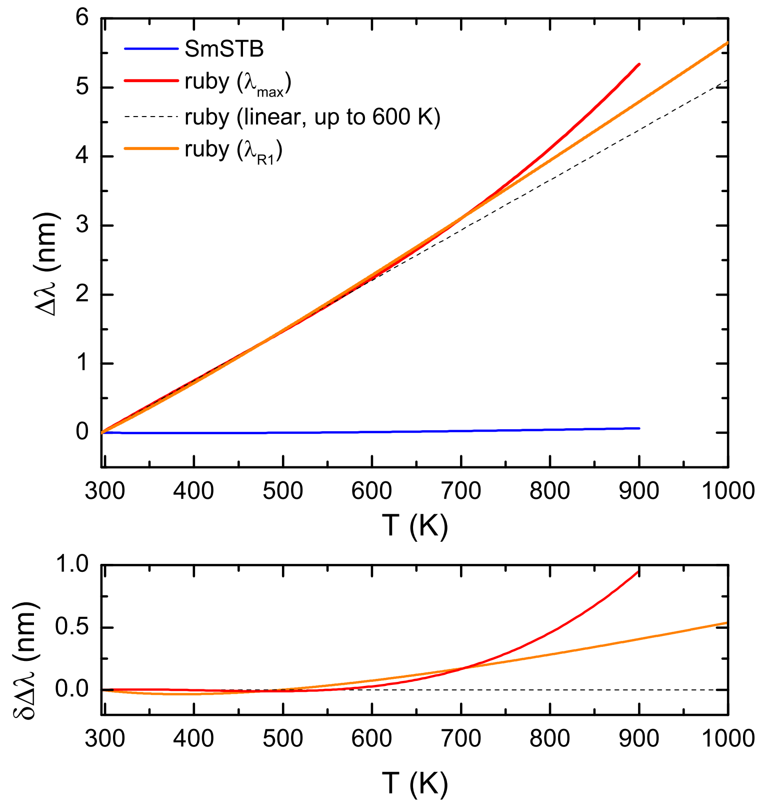
$$\nu_{R_1}(T) = \nu_{R_1}(0) + \alpha_{R_1}\left(\frac{T}{\Theta_{D,R_1}}\right)^4 \int_0^{\Theta_{D,R_1}/T} \frac{x^3}{e^x - 1} dx,$$

with

$$\nu_{R_1}(0) = \frac{10^7}{\lambda_{00}}$$

where $\lambda_{00} = \lambda_{T0,P0} - 0.8871553$ nm and $\lambda_{T0,P0} = 694.281$ nm. α_{R1} = -413 cm^{-1}, and the Debye temperature is Θ_{D,R_1}=760 K. The parameter α_{R_1} is different in McCumber [4] where α_{R_1}=-400 cm^{-1}. The difference comes from an approximate inclusion of the third and fourth terms of Eq. (3a) in Ref. [4]. The shift in λ (nm) as a function of T is finally :

$$\Delta\lambda_{R_1}(T) = \frac{10^7}{\nu_{R_1}(T)}.$$



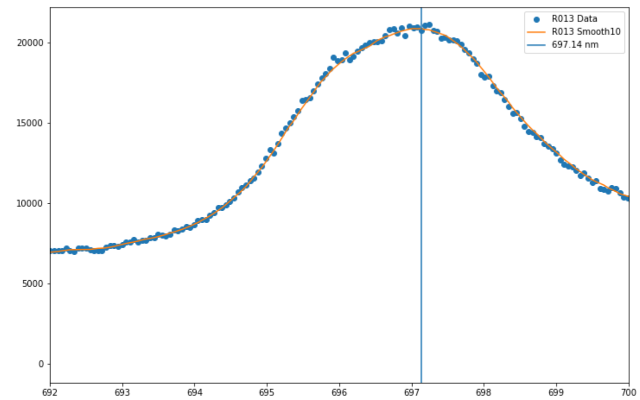
Supplementary Figure S2. Dependence of the wavelength shift $\Delta\lambda$ as a function of T, for SmSTB (blue line) and ruby, with 3 models : linear up to 600 K (dashed black line), Datchi model discussed in Sec. III A using λ_{max} (red line) and McCumber model discussed in Sec. III B λ_{R_1} (orange curve). The linear relation is $\Delta\lambda(nm) = 0.00726\,(T(K) - 296)$ (see Eq.(1) in Ref. [2]). The lower panel shows the difference between $\Delta\lambda(T)$ and the linear relation.

[1] S. Ayrinhac, M. Gauthier, M. Morand, Y. Garino, S. Boccato, F. Decremps, P. Parisiades, P. Rosier, N. C. Siersch, A. Seghour, *et al.*, Determination of indium melting curve at high pressure by picosecond acoustics, Physical Review Materials **6**, 063403 (2022).

[2] F. Datchi, A. Dewaele, P. Loubeyre, R. Letoullec, Y. Le Godec, and B. Canny, Optical pressure sensors for high-pressure–high-temperature studies in a diamond anvil cell, High Pressure Research **27**, 447 (2007).

[3] K. Syassen, Ruby under pressure, High Pressure Research **28**, 75 (2008).

[4] D. McCumber and M. Sturge, Linewidth and temperature shift of the r lines in ruby, Journal of Applied Physics **34**, 1682 (1963).



Supplementary Figure S3. Example of a ruby spectra (blue points) which is smoothed (orange line) to extract the position of the maximum λ_{max} (blue vertical line).