

แบบจำลองการดูดกลืนแสงของซิลิคอนรูพรุน

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A MODEL FOR OPTICAL ABSORPTION OF POROUS SILICON

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เราได้จำลองซิลิคอนรูพรุน ให้เป็นระบบไร้ระเบียบซึ่งประกอบด้วยหลุมศักย์สามมิติซึ่งมีการกระจายอย่างสุ่ม หลุมศักย์เหล่านี้เกิดขึ้นจากการนำอะตอมของซิลิคอนบางส่วนออกไปอย่างสุ่มจากผลึกสมบูรณ์ของซิลิคอน เราสามารถหาสมการเชิงวิเคราะห์ของความหนาแน่นสถานะเชิงอิเล็กทรอนิกส์ได้โดยการใช้เทคนิคการอินทิเกรตตามวิถีของฟายน์แมนสำหรับระบบไร้ระเบียบ การกระเพื่อมของศักย์อย่างสุ่มนี้เป็นสาเหตุทำให้เกิดสถานะเฉพาะถิ่นในส่วนหางของแถบพลังงานและทำให้ช่องว่างแถบพลังงานกว้างขึ้นด้วย การกว้างขึ้นของช่องว่างแถบพลังงานนี้สามารถสังเกตได้จากช่องว่างสภาพเคลื่อนที่ได้ของซิลิคอนรูพรุนและสามารถประเมินได้ว่าเป็นฟังก์ชันของค่าความพรุน เราได้คำนวณค่าสัมประสิทธิ์การดูดกลืนเชิงแสงสำหรับค่าความพรุนโดยใช้แบบจำลองการดูดกลืนอย่างง่ายร่วมกับความหนาแน่นสถานะที่ได้จากการคำนวณเพื่อที่จะพิจารณาช่วงของพลังงานที่การดูดกลืนเชิงแสงมีส่วนเกี่ยวข้องอย่างมีนัยสำคัญกับการเปลี่ยนสถานะโดยไม่มีโฟนอนมาเกี่ยวข้อง ผลจากการคำนวณชี้ให้เห็นว่าในการดูดกลืนเชิงแสงนั้นเราสามารถละทิ้งผลจากการเปลี่ยนสถานะโดยไม่มีโฟนอนมาเกี่ยวข้องได้อย่างมีเหตุผล นอกจากนี้เรายังวิเคราะห์ค่าความแรงของตัวกระเจิงประกอบกับผลการคำนวณการดูดกลืนเชิงแสงซึ่งแสดงให้เห็นถึงบทบาทที่สำคัญของการแจกแจงขนาดของผลึกขนาดนาโนเมตรในซิลิคอนรูพรุน

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We model porous silicon as a disordered system assembled of random distributing three-dimensional quantum wells produced from random removals of some silicon atoms from a perfect crystalline silicon. An analytic expression for its electronic density of states is determined using Feynman's path integral technique for disordered systems. Random fluctuations generated from disorder of the system create localized states in band tails as well as band-gap widening. The latter effect could be observed from the mobility gap of porous silicon, and can roughly be estimated as a function of its porosity. Optical absorption coefficients with various values of porosity are determined using the obtained density of states and a simple absorption model in order to investigate the energy range which significantly involves with non-phonon assisted transitions. The calculation indicates that non-phonon assisted processes can reasonably be neglected in optical absorption calculation for all values of porosity of studies. The important role of nanocrystal size distribution of porous silicon is also emphasized in the calculation as well as examination of scatterer strength.

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